

D-OPTIMAL DESIGNS WITH ORDERED CATEGORICAL DATA

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Abstract: Cumulative link models have been widely used for ordered categorical responses. Uniform allocation of experimental units is commonly used in practice, but often suffers from a lack of efficiency. We consider D-optimal designs with ordered categorical responses and cumulative link models. For a predetermined set of design points, we derive the necessary and sufficient conditions for an allocation to be locally D-optimal and develop efficient algorithms for obtaining approximate and exact designs. We prove that the number of support points in a minimally supported design only depends on the number of predictors, which can be much less than the number of parameters in the model. We show that a D-optimal minimally supported allocation in this case is usually not uniform on its support points. In addition, we provide EW D-optimal designs as a highly efficient surrogate to Bayesian D-optimal designs. Both of them can be much more robust than uniform designs.

Key words and phrases: Approximate design, exact design, multinomial response, cumulative link model, minimally supported design, ordinal data.

1. Introduction

In this paper we determine optimal and efficient designs for factorial experiments with qualitative factors and ordered categorical responses, or simply ordinal data. Design of experiment with multinomial response, and ordered categories in particular, is becoming increasingly popular in a rich variety of scientific disciplines especially when human evaluations are involved (Christensen, 2015). Examples include wine bitterness study (Randall, 1989), potato pathogen experiments (Omer et al., 2000), radish seedling's damping-off study (Krause et al., 2001), polysilicon deposition study (Wu, 2008), beef cattle research (Osterstock et al., 2010), and toxicity study (Agresti, 2013).

This research is motivated by an *odor removal study* conducted by the textile engineers at the University of Georgia. The scientists studied the manufacture of bio-plastics containing odorous volatiles, which need to be removed before commercialization. For that purpose, a 2^2 factorial experiment was conducted using algae and synthetic plastic resin blends. The two factors are **types of algae** (x_1 : raffinated or solvent extracted algae (−), catfish pond algae (+)) and **synthetic resins** (x_2 : polyethylene (−),

polypropylene (+)). The response Y has three ordered categories: serious odor ($j = 1$), medium odor ($j = 2$), and almost no odor ($j = 3$). Following the traditional factorial design theory, a pilot study with equal number (10 in this case) of replicates at each experimental setting was conducted, known as a *uniform design*. The results are summarized in Table 1, where y_{ij} represents the number of responses falling into the j th category under the i th experimental setting. As demonstrated later (Section 4), the best design identified by our research could improve the efficiency by 25% with only three experimental settings involved.

Table 1: Pilot Study of Odor Removal Study

Experimental setting i	Factor level		Summarized responses (Y , odor)		
	Algae x_1	Resin x_2	Serious y_{i1}	Medium y_{i2}	No odor y_{i3}
1	+	+	2	6	2
2	+	−	7	2	1
3	−	+	0	0	10
4	−	−	0	2	8

For such kind of ordinal response Y with J categories and d predictors $\mathbf{x} = (x_1, \dots, x_d)^T$, the most popular model in practice was the *proportional odds model* (also known as *cumulative logit model*, see Liu and Agresti (2005) for a detailed review). McCullagh (1980) extended it into the *cumulative link model* (also known as *ordinal regression model*)

$$g(P(Y \leq j \mid \mathbf{x})) = \theta_j - \boldsymbol{\beta}^T \mathbf{x}, \quad j = 1, \dots, J - 1 \quad (1.1)$$

where g is a general link function. The proportional odds model is a special case when g is the logit link. Nevertheless, link functions other than logit may fit some experiments better. Examples include the complementary log-log link for the polysilicon deposition study (see Example 4.6) and the cauchit link for the toxicity study (see Example 5.9). In this paper, we adopt the cumulative link model (1.1).

When there are only two categories ($J = 2$), the cumulative link model (1.1) is essentially a generalized linear model for binary data (McCullagh and Nelder, 1989; Dobson and Barnett, 2008). For optimal designs under generalized linear models, there is a growing body of literature (see Khuri et al. (2006), Atkinson et al. (2007), Stufken and Yang (2012) and references therein). In this case, it is known that the minimum number of experimental settings required by a nondegenerate Fisher information

matrix is $d + 1$, which equals the number of parameters (Fedorov, 1972; Yang and Mandal, 2015). A design with the least number of experimental settings, known as a *minimally supported design*, is of practical significance with a specified regression model due to the cost of changing settings. It is also known that the experimental units should be uniformly assigned when a minimally supported design is adopted for binary response or under a univariate generalized linear model (Yang and Mandal, 2015).

When $J \geq 3$, the cumulative link model should rather be treated as a special case of the multivariate generalized linear model (McCullagh, 1980). The relevant results in the optimal design literature are meagre and restricted to the logit link function (Zocchi and Atkinson, 1999; Perevozskaya et al., 2003). In this paper, we obtain both theoretical results and efficient algorithms for general link functions and reveal that the optimal designs with $J \geq 3$ are quite different from the cases with $J = 2$. We prove that the minimum number of experimental settings is still $d + 1$ but strictly less than the number of parameters $d + J - 1$ (Theorems 2.3 and 2.4). This counter-intuitive result is due to the multinomial-type responses: from a single experimental setup, the summarized responses have $J - 1$ degrees of freedom, requiring fewer number of distinct experimental settings in a minimally supported design. Because of the same reason, the allocation of replicates in a minimally supported design is usually not uniform either (Section 5), which is different from the traditional factorial design theory.

Similar to the cases of generalized linear models, the information matrix under cumulative link models depends on unknown parameters. In the literature, different approaches have been proposed to solve the dependence of optimal designs on unknown parameters, including local optimality (Chernoff, 1953), Bayesian approach (Chaloner and Verdinelli, 1995), maximin approach (Pronzato and Walter, 1988; Imhof, 2001), and sequential procedure (Ford et al., 1989). As pointed out by Ford, Torsney, and Wu (1992), locally optimal designs are not only important when good initial parameters are available from previous experiments, but can also be a benchmark for designs chosen to satisfy experimental constraints. In this paper, we mainly focus on locally optimal designs. For situations where local values of the parameters are difficult to obtain but the experimenter has an idea of the range of parameters with or without a prior distribution, we recommend EW optimal designs, where the Fisher information matrix is replaced by its expected values (Atkinson et al., 2007; Yang, Mandal, and Majumdar, 2016). We compare Bayesian D-optimal designs (Chaloner and Verdinelli, 1995) with EW D-optimal designs for ordinal data. As a surrogate for Bayesian designs, EW design is much easier to find and retains high efficiency with respect to Bayesian criterion (Section 6).

Among various optimal design criteria, D-optimality, which maximizes the determinant of Fisher information matrix, is the most frequently used one (Zocchi and Atkinson, 1999) and often performs well according to other criteria (Atkinson et al., 2007). In this paper, we study D-optimal designs.

In the design literature, one type of experiments deal with quantitative or continuous factors only. Such a design problem includes identification of a set of design points $\{\mathbf{x}_i\}_{i=1,\dots,m}$ and the corresponding weights $\{p_i\}_{i=1,\dots,m}$ (see, for example, Atkinson et al. (2007) and Stufken and Yang (2012)). For this type of optimal design problems, numerical algorithms are typically used for cases with two or more factors (see, for example, Woods et al. (2006)). Another type of experiments employ qualitative or discrete factors, where the set of design points $\{\mathbf{x}_i\}_{i=1,\dots,m}$ is predetermined and only the weights $\{p_i\}_{i=1,\dots,m}$ are to be optimized (see, for example, Yang and Mandal (2015)). One connection between the two types of designs is that one can pick up grid points of the continuous factors and turn the first-type problems into the second. Tong, Volkmer, and Yang (2014, Section 5) also bridged the gap between the two types of problems in a way that the results involving discrete factors can be applied to the cases with continuous factors as well. In this paper, we concentrate on the second type of design problems and assume that $\{\mathbf{x}_i\}_{i=1,\dots,m}$ are given and fixed.

This paper is organized as follows. In Section 2, we describe the preliminary setup and obtain the Fisher information matrix for cumulative link model with a general link, which generalizes Perevozskaya et al. (2003)'s result for logit link. We also identify a necessary and sufficient condition for the Fisher information matrix to be positive definite, which determines the minimum number of experimental settings required. In Sections 3 and 4, we provide both theoretical results and numerical algorithms for searching locally D-optimal approximate or exact designs. In Section 5, we identify analytic D-optimal designs for special cases to illustrate that a D-optimal minimally supported design is usually not uniform on its support points. In Section 6, we illustrate by examples that the EW D-optimal design can be highly efficient with respect to Bayesian D-optimality. We make concluding remarks in Section 7 and relegate additional proofs and results to the Supplementary Materials.

2. Fisher Information Matrix and Its Determinant

Suppose there are m ($m \geq 2$) predetermined experimental settings. For the i th experimental setting with corresponding predictors $\mathbf{x}_i = (x_{i1}, \dots, x_{id})^T \in \mathbb{R}^d$ ($d \geq 1$), there are n_i experimental units assigned to it. Among the n_i experimental units, the k th one generates a response V_{ik} which belongs to one of J ($J \geq 2$) ordered categories. As shown in Example 2.2

later, the dimension d of the predictors can be significantly larger than the number of factors considered in the experiment, which allows more flexible models.

2.1 General setup

In many real applications, V_{i1}, \dots, V_{in_i} are regarded as i.i.d. discrete random variables. Denote $\pi_{ij} = P(V_{ik} = j)$, where $i = 1, \dots, m$; $j = 1, \dots, J$; and $k = 1, \dots, n_i$. Let $Y_{ij} = \#\{k \mid V_{ik} = j\}$ be the number of V_{ik} 's falling into the j th category. Then $(Y_{i1}, \dots, Y_{iJ}) \sim \text{Multinomial}(n_i; \pi_{i1}, \dots, \pi_{iJ})$. Throughout this paper, we assume

Assumption 2.1. $0 < \pi_{ij} < 1$, $i = 1, \dots, m$; $j = 1, \dots, J$.

Denote $\gamma_{ij} = P(V_{ik} \leq j) = \pi_{i1} + \dots + \pi_{ij}$, $j = 1, \dots, J$. Based on Assumption 2.1, $0 < \gamma_{i1} < \gamma_{i2} < \dots < \gamma_{i,J-1} < \gamma_{iJ} = 1$ for each $i = 1, \dots, m$. Consider independent multinomial observations (Y_{i1}, \dots, Y_{iJ}) , $i = 1, \dots, m$ with corresponding predictors $\mathbf{x}_1, \dots, \mathbf{x}_m$. Under a *cumulative link model* or *ordinal regression model* (McCullagh, 1980; Agresti, 2013; Christensen, 2015), there exists a link function g and parameters of interest $\theta_1, \dots, \theta_{J-1}, \boldsymbol{\beta} = (\beta_1, \dots, \beta_d)^T$, such that

$$g(\gamma_{ij}) = \theta_j - \mathbf{x}_i^T \boldsymbol{\beta}, \quad j = 1, \dots, J-1. \quad (2.1)$$

This leads to $m(J-1)$ equations in $d+J-1$ parameters $(\beta_1, \dots, \beta_d, \theta_1, \dots, \theta_{J-1})$. Throughout this paper, we assume

Assumption 2.2. The link g is differentiable and its derivative $g' > 0$.

Assumption 2.2 is satisfied for commonly used link functions including **logit** ($\log(\gamma/(1-\gamma))$), **probit** ($\Phi^{-1}(\gamma)$), **log-log** ($-\log(-\log(\gamma))$), **complementary log-log** ($\log(-\log(1-\gamma))$), and **cauchit** ($\tan(\pi(\gamma-1/2))$) (McCullagh and Nelder, 1989; Christensen, 2015). Some relevant formulas of these link functions are provided in the Supplementary Materials (Section S.1). According to Assumption 2.2, g is strictly increasing, and then $\theta_1 < \theta_2 < \dots < \theta_{J-1}$.

Example 2.1. Consider the logit link $g(\gamma) = \log(\gamma/(1-\gamma))$ with two predictors and three ordered categories. Model (2.1) consists of $2m$ equations $g(\gamma_{ij}) = \theta_j - x_{i1}\beta_1 - x_{i2}\beta_2$, $i = 1, \dots, m$; $j = 1, 2$ and 4 parameters $(\beta_1, \beta_2, \theta_1, \theta_2)$. Under Assumptions 2.1 and 2.2, $\theta_1 < \theta_2$. \square

Example 2.2. Suppose the model consists of three covariates x_1, x_2, x_3 and a few second-order predictors, $g(\gamma_{ij}) = \theta_j - x_{i1}\beta_1 - x_{i2}\beta_2 - x_{i3}\beta_3 - x_{i1}x_{i2}\beta_{12} - x_{i1}^2\beta_{11} - x_{i2}^2\beta_{22}$, where $i = 1, \dots, m$; $j = 1, \dots, J-1$. Then the number of predictors is $d = 6$. \square

Under the cumulative link model (2.1), the log-likelihood function (up to a constant) is $l(\beta_1, \dots, \beta_d, \theta_1, \dots, \theta_{J-1}) = \sum_{i=1}^m \sum_{j=1}^J Y_{ij} \log(\pi_{ij})$, where $\pi_{ij} = \gamma_{ij} - \gamma_{i,j-1}$ with $\gamma_{ij} = g^{-1}(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta})$ for $j = 1, \dots, J-1$ and $\gamma_{i0} = 0$, $\gamma_{iJ} = 1$.

Perevozskaya et al. (2003) obtained a detailed form of the Fisher information matrix for logit link and one predictor. Our theorem below is for general link and d predictors with proof relegated into the Supplementary Materials (Section S.3).

Theorem 2.1. *Under Assumptions 2.1 and 2.2, the Fisher information matrix can be written as*

$$\mathbf{F} = \sum_{i=1}^m n_i \mathbf{A}_i \quad (2.2)$$

where \mathbf{A}_i is a $(d + J - 1) \times (d + J - 1)$ matrix

$$\mathbf{A}_i = \begin{pmatrix} \mathbf{A}_{i1} & \mathbf{A}_{i2} \\ \mathbf{A}_{i2}^T & \mathbf{A}_{i3} \end{pmatrix} = \begin{pmatrix} (e_i x_{is} x_{it})_{s=1, \dots, d; t=1, \dots, d} & (-x_{is} c_{it})_{s=1, \dots, d; t=1, \dots, J-1} \\ (-c_{is} x_{it})_{s=1, \dots, J-1; t=1, \dots, d} & \mathbf{A}_{i3} \end{pmatrix}$$

and \mathbf{A}_{i3} is a $(J-1) \times (J-1)$ symmetric tri-diagonal matrix with diagonal entries $u_{i1}, \dots, u_{i,J-1}$ and off-diagonal entries $-b_{i2}, \dots, -b_{i,J-1}$ when $J \geq 3$, where $e_i = \sum_{j=1}^J \pi_{ij}^{-1} (g_{ij} - g_{i,j-1})^2 > 0$ with $g_{ij} = (g^{-1})'(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta}) > 0$ for $j = 1, \dots, J-1$ and $g_{i0} = g_{iJ} = 0$; $c_{it} = g_{it} [\pi_{it}^{-1} (g_{it} - g_{i,t-1}) - \pi_{i,t+1}^{-1} (g_{i,t+1} - g_{it})]$; $u_{it} = g_{it}^2 (\pi_{it}^{-1} + \pi_{i,t+1}^{-1}) > 0$; and $b_{it} = g_{i,t-1} g_{it} \pi_{it}^{-1} > 0$. Note that \mathbf{A}_{i3} contains only one entry u_{i1} when $J = 2$.

As the Fisher information matrix, \mathbf{F} is always positive semi-definite and thus $|\mathbf{F}| \geq 0$ (Fedorov, 1972). As a special case, \mathbf{A}_i is the Fisher information at the experimental setting \mathbf{x}_i (also known as a *design point* or *support point*) and thus positive semi-definite too.

2.2 Determinant of Fisher information matrix

Among different criteria for optimal designs, D-criterion looks for the allocation maximizing $|\mathbf{F}|$, the determinant of \mathbf{F} . Here, a D-optimal design with m predetermined design points $\mathbf{x}_1, \dots, \mathbf{x}_m$ could either be an integer-valued allocation (n_1, n_2, \dots, n_m) maximizing $|\mathbf{F}|$ with fixed $n = \sum_{i=1}^m n_i > 0$, known as an *exact design*; or a real-valued allocation (p_1, p_2, \dots, p_m) maximizing $|n^{-1} \mathbf{F}|$ with $p_i = n_i/n \geq 0$ and $\sum_{i=1}^m p_i = 1$, known as an *approximate design*.

Theorem 2.2. *The determinant of the Fisher information matrix*

$$|\mathbf{F}| = \sum_{\alpha_1 + \dots + \alpha_m = d + J - 1} c_{\alpha_1, \dots, \alpha_m} \cdot n_1^{\alpha_1} \cdots n_m^{\alpha_m}$$

which is an order- $(d + J - 1)$ homogeneous polynomial of (n_1, \dots, n_m) and

$$c_{\alpha_1, \dots, \alpha_m} = \sum_{\tau \in (\alpha_1, \dots, \alpha_m)} |\mathbf{A}_\tau| \quad (2.3)$$

The proof of Theorem 2.2 is relegated into the Supplementary Materials (Section S.3). Given a map $\tau : \{1, 2, \dots, d + J - 1\} \rightarrow \{1, \dots, m\}$, \mathbf{A}_τ in (2.3) is a $(d + J - 1) \times (d + J - 1)$ matrix whose k th row is the same as the k th row of $\mathbf{A}_{\tau(k)}$, $k = 1, \dots, d + J - 1$. We denote $\tau \in (\alpha_1, \dots, \alpha_m)$ if $\alpha_i = \#\{j : \tau(j) = i\}$ for each $i = 1, \dots, m$.

In order to obtain analytic properties of $|\mathbf{F}|$, we need a few lemmas including the following one, which covers Lemma 1 in Perevozskaya et al. (2003) as a special case:

Lemma 2.1. $\text{Rank}(\mathbf{A}_i) = \text{Rank}(\mathbf{A}_{i3}) = J - 1$. Furthermore, \mathbf{A}_{i3} is positive definite and

$$|\mathbf{A}_{i3}| = \prod_{s=1}^{J-1} g_{is}^2 \cdot \prod_{t=1}^J \pi_{it}^{-1} > 0$$

where $g_{is} = (g^{-1})'(\theta_s - \mathbf{x}_i^T \boldsymbol{\beta}) > 0$ for $s = 1, \dots, J - 1$.

Example 2.3. Suppose $d = 2$, $J = 3$ with link function g . According to Theorem 2.2, $|\mathbf{F}|$ in this case is an order-4 homogeneous polynomial of (n_1, \dots, n_m) . Based on Lemma S.4 and Lemma S.5 in the Supplementary Materials (Section S.2), we can remove all the terms in the form of n_i^4 , $n_i^3 n_j$, or $n_i^2 n_j^2$ from $|\mathbf{F}|$. Therefore,

$$|\mathbf{F}| = \sum_{i=1}^m \sum_{j < k, j \neq i, k \neq i} c_{ijk} \cdot n_i^2 n_j n_k + \sum_{i < j < k < l} c_{ijkl} \cdot n_i n_j n_k n_l$$

for some coefficients c_{ijk} and c_{ijkl} . \square

Based on Lemma S.4 and Lemma S.5, in order to keep $c_{\alpha_1, \dots, \alpha_m} \neq 0$, the largest possible α_i is $J - 1$ and the fewest possible number of positive α_i 's is $d + 1$. As a direct conclusion of Lemma S.5, the following theorem states that a minimally supported design has at least $d + 1$ support point, which could be much less than the number of parameters $d + J - 1$:

Theorem 2.3. *In order to keep the Fisher information matrix positive definite, we need at least $d + 1$ experimental settings. In other words, $|\mathbf{F}| > 0$ only if $m \geq d + 1$.*

In order to find out whether $d + 1$ experimental settings or support points are enough to keep the Fisher information matrix positive definite, we study the leading term of $|\mathbf{F}|$ with $\max_{1 \leq i \leq m} \alpha_i = J - 1$. For example, $\alpha_{i_0} = J - 1$ for some $1 \leq i_0 \leq m$. Due to Lemma S.5 and $\sum_{i=1}^m \alpha_i = d + J - 1$, in order to keep $c_{\alpha_1, \dots, \alpha_m} \neq 0$, there must exist $1 \leq i_1 < i_2 < \dots < i_d \leq m$ which are different from i_0 , such that, $\alpha_{i_1} = \dots = \alpha_{i_d} = 1$. The following lemma provides an explicit formula for such a coefficient $c_{\alpha_1, \dots, \alpha_m}$:

Lemma 2.2. *Suppose $\alpha_{i_0} = J - 1$ and $\alpha_{i_1} = \dots = \alpha_{i_d} = 1$. Then*

$$c_{\alpha_1, \dots, \alpha_m} = \prod_{s=1}^d e_{i_s} \cdot |\mathbf{A}_{i_0 3}| \cdot |\mathbf{X}_1[i_0, i_1, \dots, i_d]|^2$$

where $\mathbf{X}_1 = (\mathbf{1} \ \mathbf{X})$ is an $m \times (d + 1)$ matrix with $\mathbf{1} = (1, \dots, 1)^T$, $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_m)^T$, and $\mathbf{X}_1[i_0, i_1, \dots, i_d]$ is the sub-matrix consisting of the i_0 th, i_1 th, \dots , i_d th rows of \mathbf{X}_1 .

The proof for Lemma 2.2 is relegated to the Supplementary Materials (Section S.3). For the purpose of finding D-optimal allocations, we write $|\mathbf{F}| = f(n_1, \dots, n_m)$ for an order- $(d + J - 1)$ homogeneous polynomial function f . The *D-optimal exact design problem* is to find an integer-valued allocation (n_1, \dots, n_m) maximizing $f(n_1, \dots, n_m)$ subject to $n_i \in \{0, 1, \dots, n\}$, $i = 1, \dots, m$ and $n_1 + \dots + n_m = n$ with given positive integer n . Denote $p_i = n_i/n$, $i = 1, \dots, m$. According to Theorem 2.1,

$$f(n_1, \dots, n_m) = \left| \sum_{i=1}^m n_i \mathbf{A}_i \right| = \left| n \sum_{i=1}^m p_i \mathbf{A}_i \right| = n^{d+J-1} f(p_1, \dots, p_m) \quad (2.4)$$

Due to (2.4), Theorems 2.2 and 2.3 can be directly applied to approximate designs too, while the *D-optimal approximate design problem* is to find a real-valued allocation (p_1, \dots, p_m) maximizing $f(p_1, p_2, \dots, p_m)$ subject to $0 \leq p_i \leq 1$, $i = 1, \dots, m$ and $p_1 + \dots + p_m = 1$.

According to Lemma 2.1, $|\mathbf{A}_{i_0 3}| > 0$. Thus $c_{\alpha_1, \dots, \alpha_m}$ in Lemma 2.2 is positive as long as $\mathbf{X}_1[i_0, \dots, i_d]$ is of full rank. Theorem 2.3 implies that a minimally supported design contains at least $d + 1$ support points, while the following theorem states a necessary and sufficient condition for the minimum number of support points to be exactly $d + 1$:

Theorem 2.4. *The Fisher information matrix is positive definite for some approximate design if and only if the extended design matrix $\mathbf{X}_1 = (\mathbf{1} \ \mathbf{X})$ is of full rank. In other words, $f(\mathbf{p}) > 0$ for some $\mathbf{p} = (p_1, \dots, p_m)^T$ if and only if $\text{Rank}(\mathbf{X}_1) = d + 1$.*

The result stated in Theorem 2.4 appears to be mysterious at the first sight, since it claims that the minimal number of experimental settings required could be strictly less than the number of parameters. We use the motivating example presented in Table 1 to interpret the reason. In the odor removal study, the main-effects cumulative link model (2.1) involves four independent parameters – two β 's for the covariates ($d = 2$) and two θ 's for the intercepts ($J - 1 = 2$). According to Theorem 2.4, a minimally supported design may involve only three experimental settings. This apparent anomaly is due to the fact that, for multinomial responses with $J = 3$ categories, we get two degrees of freedom (i.e., Y_{i1}, Y_{i2}) from each experimental setting. Due to the same reason, the optimal allocation of experimental units is often not uniform (see Section 4), contrary to the case of binary responses (Yang, Mandal, and Majumdar, 2016; Yang and Mandal, 2015).

3. D-optimal Approximate Design

A (locally) D-optimal approximate design is a real-valued allocation $\mathbf{p} = (p_1, \dots, p_m)^T$ maximizing $f(\mathbf{p}) = f(p_1, \dots, p_m)$ with pre-specified values of parameters. The solution always exists since f is continuous and the set of feasible allocations $S := \{(p_1, \dots, p_m)^T \in \mathbb{R}^m \mid p_i \geq 0, i = 1, \dots, m; \sum_{i=1}^m p_i = 1\}$ is convex and compact. Theorem 2.4 ascertains that a nontrivial D-optimal approximate design problem needs the following assumption:

Assumption 3.3. There are at least $d+1$ experimental settings and the extended design matrix \mathbf{X}_1 is of full rank. In other words, $m \geq d+1$ and $\text{Rank}(\mathbf{X}_1) = d+1$.

Assumption 3.3 is assumed for the rest of the paper. Then the set of *valid* allocations $S_+ := \{\mathbf{p} = (p_1, \dots, p_m)^T \in S \mid f(\mathbf{p}) > 0\}$ is nonempty. Since $\mathbf{F} = \sum_{i=1}^m n_i \mathbf{A}_i = n \sum_{i=1}^m p_i \mathbf{A}_i$ is linear in \mathbf{p} and $\phi(\cdot) = \log |\cdot|$ is concave on positive semi-definite matrices, then $f(\mathbf{p}) = n^{1-d-J} |\mathbf{F}|$ is log-concave (Silvey, 1980) and thus S_+ is also convex. The following theorem characterizes all valid allocations in terms of the extended design matrix \mathbf{X}_1 :

Theorem 3.5. A feasible allocation $\mathbf{p} = (p_1, \dots, p_m)^T$ satisfies $f(\mathbf{p}) > 0$ if and only if $\text{Rank}(\mathbf{X}_1[\{i \mid p_i > 0\}]) = d+1$, where $\mathbf{X}_1[\{i \mid p_i > 0\}]$ is the sub-matrix consisting of the $\{i \mid p_i > 0\}$ th rows of \mathbf{X}_1 . In other words, $S_+ = \{\mathbf{p} = (p_1, p_2, \dots, p_m)^T \in S \mid \text{Rank}(\mathbf{X}_1[\{i \mid p_i > 0\}]) = d+1\}$.

As a direct conclusion of Theorem 3.5, S_+ contains all \mathbf{p} whose coordinates are all strictly positive. A special case is the uniform allocation $\mathbf{p}_u = (1/m, \dots, 1/m)^T$.

A necessary and sufficient condition for an approximate design to be D-optimal is of the general-equivalence-theorem type (Kiefer, 1974; Pukelsheim,

1993; Atkinson et al., 2007; Stufken and Yang, 2012; Fedorov and Leonov, 2014; Yang, Mandal, and Majumdar, 2016), which is convenient when searching for numerical solutions. Following Yang, Mandal, and Majumdar (2016), for a given $\mathbf{p} = (p_1, \dots, p_m)^T \in S_+$ and $i \in \{1, \dots, m\}$, we define

$$f_i(z) = f\left(\frac{1-z}{1-p_i}p_1, \dots, \frac{1-z}{1-p_i}p_{i-1}, z, \frac{1-z}{1-p_i}p_{i+1}, \dots, \frac{1-z}{1-p_i}p_m\right) \quad (3.1)$$

with $0 \leq z \leq 1$. Note that $f_i(z)$ is well defined as long as $p_i < 1$. Following the proof of Theorem 2.4, we obtain the next theorem on the coefficients of $f_i(z)$:

Theorem 3.6. *Suppose $\mathbf{p} = (p_1, \dots, p_m)^T \in S_+$ and $i \in \{1, \dots, m\}$. For $0 \leq z \leq 1$,*

$$f_i(z) = (1-z)^d \sum_{j=0}^{J-1} a_j z^j (1-z)^{J-1-j} \quad (3.2)$$

where $a_0 = f_i(0)$, $(a_{J-1}, \dots, a_1)^T = \mathbf{B}_{J-1}^{-1} \mathbf{c}$, $\mathbf{B}_{J-1} = (s^{t-1})_{st}$ is a $(J-1) \times (J-1)$ matrix, and $\mathbf{c} = (c_1, \dots, c_{J-1})^T$ with $c_j = (j+1)^{d+J-1} j^{-d} f_i(1/(j+1)) - j^{J-1} f_i(0)$.

Following the lift-one algorithm proposed in Yang, Mandal, and Majumdar (2016), we have parallel results and algorithm for our case. For simplicity, we also call our algorithm *lift-one algorithm*.

Theorem 3.7. *Given an allocation $\mathbf{p} = (p_1^*, \dots, p_m^*)^T \in S_+$, \mathbf{p} is D -optimal if and only if for each $i = 1, \dots, m$, $f_i(z)$, $0 \leq z \leq 1$ attains its maximum at $z = p_i^*$.*

Our lift-one algorithm:

- 1° Start with an allocation $\mathbf{p}_0 = (p_1, \dots, p_m)^T$ satisfying $f(\mathbf{p}_0) > 0$.
- 2° Set up a random order of i going through $\{1, 2, \dots, m\}$.
- 3° For each i , determine $f_i(z)$ according to Theorem 3.6 with J determinants $f_i(0), f_i(1/2), f_i(1/3), \dots, f_i(1/J)$ calculated according to (3.1).
- 4° Use quasi-Newton method with gradient defined in (S.13) to find z_* maximizing $f_i(z)$ with $0 \leq z \leq 1$. If $f_i(z_*) \leq f_i(0)$, let $z_* = 0$. Define $\mathbf{p}_*^{(i)} = (p_1(1-z_*)/(1-p_i), \dots, p_{i-1}(1-z_*)/(1-p_i), z_*, p_{i+1}(1-z_*)/(1-p_i), \dots, p_m(1-z_*)/(1-p_i))^T$. Note that $f(\mathbf{p}_*^{(i)}) = f_i(z_*)$.
- 5° Replace \mathbf{p}_0 with $\mathbf{p}_*^{(i)}$, and $f(\mathbf{p}_0)$ with $f(\mathbf{p}_*^{(i)})$.
- 6° Repeat 2° ~ 5° until convergence, that is, $f(\mathbf{p}_0) = f(\mathbf{p}_*^{(i)})$ for each i .

Theorem 3.8. *When the lift-one algorithm converges, the resulting \mathbf{p} maximizes $f(\mathbf{p})$.*

Example 3.4. Odor removal study In our motivating example (Section 1), the response was ordinal in nature, **serious odor**, **medium odor**, and **no odor**. We consider the logit link and fit the cumulative link model (2.1) to the data presented in Table 1. The estimated values of the model parameters are $(\hat{\beta}_1, \hat{\beta}_2, \hat{\theta}_1, \hat{\theta}_2)^T = (-2.44, 1.09, -2.67, -0.21)^T$. Suppose a follow-up experiment is planned and the estimated parameter values are regarded as the true value. The D-optimal approximate allocation found by the lift-one algorithm is $\mathbf{p}_o = (0.4449, 0.2871, 0, 0.2680)^T$. The efficiency of the uniform one $\mathbf{p}_u = (1/4, 1/4, 1/4, 1/4)^T$ is $(f(\mathbf{p}_u)/f(\mathbf{p}_o))^{1/4} = 79.7\%$ which is far from satisfactory. \square

Example 3.5. Wine bitterness study Christensen (2015, Table 1) aggregated the wine data from Randall (1989). It contains the output of a factorial experiment with two treatment factors each at two levels (**Temperature** x_1 : cold (−) or warm (+); **Contact** x_2 : no (−) or yes (+)) affecting wine bitterness. The response was ordinal with five levels (from “1” being least bitter to “5” being most bitter). The original design employed a uniform allocation $\mathbf{p}_u = (1/4, 1/4, 1/4, 1/4)^T$. The estimated parameter values under the logit link are $(\hat{\beta}_1, \hat{\beta}_2, \hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3, \hat{\theta}_4)^T = (1.25, 0.76, -3.36, -0.76, 1.45, 2.99)^T$. If a follow-up experiment is planned regarding the estimated values of the parameters as the true values, then the D-optimal approximate allocation found by the lift-one algorithm is $\mathbf{p}_o = (0.2694, 0.2643, 0.2333, 0.2330)^T$. The efficiency of the original design \mathbf{p}_u is 99.9%. Nevertheless, the corresponding efficiency may drop to 80% if $|\beta_1|$ and $|\beta_2|$ are both larger than 3 (see Figure 1(a)). In that case, the D-optimal allocations are minimally supported, that is, some p_i is 0 (see Figure 1(b)), which will be discussed further in Section 5. \square

With all examples that we study, the lift-one algorithm often converges within a few iterations. Yang, Mandal, and Majumdar (2016) also provided a modified lift-one algorithm, which is guaranteed to converge. The same procedure could be easily applied to the lift-one algorithm here if it does not converge in a pre-specified number of iterations.

4. D-optimal Exact Design

A (locally) D-optimal exact design is an integer-valued allocation $\mathbf{n} = (n_1, \dots, n_m)^T$ maximizing $|\mathbf{F}|$ with given parameter values and a pre-specified total number n of experimental units or runs. In the design literature, different discretization methods have been proposed to round an approximate design into an exact design for a given n , including the quota method (Kiefer, 1971; Pukelsheim, 1993) and the efficient rounding procedure (Pukelsheim, 1993; Pukelsheim and Rieder, 1992), which usually work well for large enough n but with no guarantee for small sample size (Imhof, Lopez-Fidalgo, and Wong, 2001).

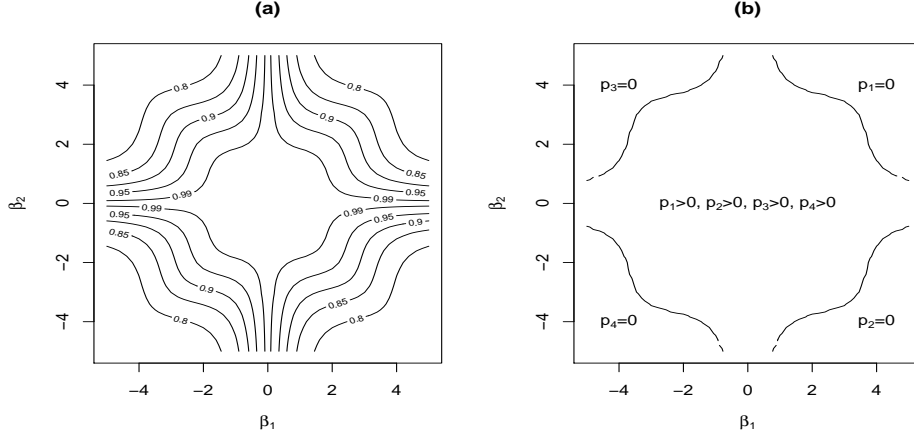


Figure 1: Wine bitterness study with assumed true parameter values $(\beta_1, \beta_2, -3.36, -0.76, 1.45, 2.99)^T$: (a) contour plot of efficiency of the original design; (b) regions for a D-optimal design to be minimally supported, that is, $p_i = 0$ for $i = 1, 2, 3$, or 4 .

In this section, we aim to provide a direct search for D-optimal exact designs. As a conclusion of Theorem 3.5, the following corollary implies that we need at least $d + 1$ experimental units to make $|\mathbf{F}| > 0$ possible:

Corollary 4.1. $|\mathbf{F}| > 0$ if and only if $\text{Rank}(\mathbf{X}_1[\{i \mid n_i > 0\}]) = d + 1$.

In order to avoid trivial cases, we assume $n \geq d + 1$ throughout this section. To maximize $f(\mathbf{n}) = f(n_1, \dots, n_m) = |\mathbf{F}|$, we adopt the idea of exchange algorithm which was first suggested by Fedorov (1972). The exchange algorithm used here is to adjust n_i and n_j simultaneously for randomly chosen (i, j) while keeping $n_i + n_j = c$ as a constant.

We start with an $\mathbf{n} = (n_1, \dots, n_m)^T$ satisfying $f(\mathbf{n}) > 0$. Following Yang, Mandal, and Majumdar (2016), for $1 \leq i < j \leq m$, we define

$$f_{ij}(z) = f(n_1, \dots, n_{i-1}, z, n_{i+1}, \dots, n_{j-1}, c - z, n_{j+1}, \dots, n_m) \quad (4.1)$$

where $c = n_i + n_j$, $z = 0, 1, \dots, c$. Note that $f_{ij}(n_i) = f(\mathbf{n})$. From Theorem 2.2, Lemmas S.4 and S.5, we obtain the following formula on calculating $f_{ij}(z)$:

Theorem 4.9. Suppose $\mathbf{n} = (n_1, \dots, n_m)^T$ satisfies $f(\mathbf{n}) > 0$ and $n_i + n_j \geq J$ for given $1 \leq i < j \leq m$. For $z = 0, 1, \dots, n_i + n_j$,

$$f_{ij}(z) = \sum_{s=0}^J c_s z^s \quad (4.2)$$

where $c_0 = f_{ij}(0)$, and c_1, \dots, c_J can be obtained using $(c_1, \dots, c_J)^T = \mathbf{B}_J^{-1}(d_1, \dots, d_J)^T$ with $\mathbf{B}_J = (s^{t-1})_{st}$ as a $J \times J$ matrix and $d_s = (f_{ij}(s) - f_{ij}(0))/s$.

Note that the $J \times J$ matrix \mathbf{B}_J in Theorem 4.9 shares the same form of \mathbf{B}_{J-1} in Theorem 3.6. According to Theorem 4.9, in order to maximize $f_{ij}(z)$ with $z = 0, 1, \dots, n_i + n_j$, one can obtain the exact polynomial form of $f_{ij}(z)$ by calculating $f_{ij}(0), f_{ij}(1), \dots, f_{ij}(J)$. There is no practical need to find out the exact form of $f_{ij}(z)$ if $n_i + n_j < J$ since one may simply calculate $f_{ij}(z)$ for each z . Following Yang, Mandal, and Majumdar (2016), an exchange algorithm (see the Supplementary Materials, Section S.5) based on Theorem 4.9 could be used to search for a D-optimal exact allocation.

Example 3.4 Odor removal study (continued) Suppose we want to conduct a follow-up experiment with n experimental units. Using the exchange algorithm mentioned above, we obtain the D-optimal exact designs across different n 's (Table 2). As expected, the D-optimal exact allocations $(n_1, \dots, n_4)^T$

Table 2: D-optimal Exact Designs and Approximate Design for Odor Removal Study

n	n_1	n_2	n_3	n_4	$n^{-4} \mathbf{F} $	# iterations	Time(sec.)
3	1	1	0	1	0.0002911	1	< 0.01
10	4	3	0	3	0.0003133	3	0.02
40	18	11	0	11	0.0003177	3	0.02
100	44	29	0	27	0.0003180	4	0.05
1000	445	287	0	268	0.0003181	5	0.39
\mathbf{p}_o	0.4449	0.2871	0	0.2680	0.0003181	5	0.03

is consistent with the D-optimal approximate allocation $\mathbf{p}_o = (p_1, \dots, p_4)^T$ (last row of Table 2) for large n . The time costs in seconds (last column of Table 2) are recorded on a PC with 2GHz CPU and 8GB memory. Suppose we rerun an experiment with $n = 40$. With respect to the D-optimal exact design $\mathbf{n}_o = (18, 11, 0, 11)^T$, the efficiency of the uniform design $\mathbf{n}_u = (10, 10, 10, 10)^T$ is $(f(\mathbf{n}_u)/f(\mathbf{n}_o))^{1/4} = 79.7\%$ only. \square

Example 4.6. Polysilicon deposition study Wu (2008) considered an experiment for studying the polysilicon deposition process with six 3-level factors, described in details by Phadke (1989). Due to the inconvenience of counting the number of surface defects, which is one of the major evaluating characteristics, they treated it as a 5-category ordinal variable: 1 for 0 ~ 3 defects, 2 for 4 ~ 30, 3 for 31 ~ 300, 4 for 301 ~ 1000, and 5 for 1001 and more. The original design, denoted by \mathbf{n}_u , includes 18 experimental settings based on the L_{18} orthogonal array. In order to apply a cumulative link model, we represent each 3-level factor, say A with levels 1, 2, 3, by its linear component A_1 taking values $-1, 0, 1$ and quadratic component A_2 taking values $1, -2, 1$ (Wu and Hamada, 2009). Then

the fitted model with complementary log-log link chosen by both AIC and BIC criteria (see, for example, Agresti (2013)) involves 4 cut-points $(\hat{\alpha}_1, \hat{\alpha}_2, \hat{\alpha}_3, \hat{\alpha}_4) = (-1.59, -0.58, 0.41, 1.22)$ and 12 other coefficients $(\hat{\beta}_{11}, \hat{\beta}_{12}, \hat{\beta}_{21}, \hat{\beta}_{22}, \dots, \hat{\beta}_{62}) = (1.45, -0.22, 1.35, 0.02, -0.12, -0.34, 0.19, 0.00, 0.22, 0.08, 0.05, 0.17)$. When a follow-up experiment is conducted and the true parameter values are assumed to be the estimated ones, we use the exchange algorithm and find out a D-optimal 18-run design, denoted by \mathbf{n}_o (see the Supplementary Materials, Section S.6, for a list of the 18 experimental settings). Compared with \mathbf{n}_o , the efficiency of the original design \mathbf{n}_u is $(f(\mathbf{n}_u)/f(\mathbf{n}_o))^{1/16} = 73.1\%$ only. In order to check the efficiency of a rounded design, we use the lift-one algorithm and find out that the D-optimal approximate design contains 100 positive p_i 's out of the 729 distinct experimental settings. In this case, both the quota method and the efficient rounding procedure end with the same rounded design \mathbf{n}_r (see Section S.6). Not unexpectedly, its efficiency is $(f(\mathbf{n}_r)/f(\mathbf{n}_o))^{1/16} = 86.1\%$ only. \square

5. Minimally Supported Design

A minimally supported design is a design with the minimal number of support points (i.e., \mathbf{x}_i with $p_i > 0$ or $n_i > 0$) while keeping the Fisher information matrix positive definite, that is, $|\mathbf{F}| > 0$. It is of practical significance since the experiment runs with the minimal number of different settings. For example, the 18 experimental settings in the polysilicon deposition study (Example 4.6) had to be run in a sequential way and only two settings were arranged in each day (Phadke, 1989). It is usually relatively easier to repeat the experiments with the same setting. Less experimental settings often indicate less time and less cost. Another practical application of a minimally supported design is to serve as the initial design for numerical searching algorithms. Since the objective function in this case takes a much simpler form, an optimal allocation restricted to those support points can be obtained more easily or even analytically.

According to Theorem 2.3, a minimally supported design contains at least $d+1$ support points. On the other hand, according to Theorem 3.5 and Corollary 4.1, a minimally supported design could contain exactly $d+1$ support points if the extended design matrix $\mathbf{X}_1 = (\mathbf{1} \ \mathbf{X})$ is of full rank, that is, $\text{Rank}(\mathbf{X}_1) = d+1$.

Example 5.7. Let $J = 2$ and then the multinomial response is actually binomial. In this case, there are $d+1$ parameters, $\theta_1, \beta_1, \dots, \beta_d$. For a general link function g satisfying Assumptions 2.1 and 2.2, $g_{i0} = g_{i2} = 0$, $g_{i1} = (g^{-1})'(\theta_1 - \mathbf{x}_i^T \boldsymbol{\beta}) > 0$, $e_i = u_{i1} = c_{i1} = g_{i1}^2 / [\pi_{i1}(1 - \pi_{i1})]$, $i = 1, \dots, m$. Then \mathbf{A}_{i3} in Theorem 2.1 contains only one entry, u_{i1} , and thus $|\mathbf{A}_{i3}| = u_{i1}$ or simply e_i (Lemma 2.1 still holds). Assume further that the $m \times d$ design matrix \mathbf{X} satisfies Assumption 3.3.

According to Theorem 2.2, Lemmas S.4, S.5, and 2.2, given $\mathbf{p} = (p_1, \dots, p_m)^T$,

$$f(\mathbf{p}) = n^{-(d+1)} |\mathbf{F}| = \sum_{1 \leq i_0 < i_1 < \dots < i_d \leq m} |\mathbf{X}_1[i_0, i_1, \dots, i_d]|^2 p_{i_0} e_{i_0} p_{i_1} e_{i_1} \dots p_{i_d} e_{i_d} \quad (5.1)$$

Note that (5.1) is essentially the same as Lemma 3.1 in Yang and Mandal (2015). Then a minimally supported design may contain $d + 1$ support points and a D-optimal one keeps equal weight $1/(d+1)$ on all support points (Yang and Mandal, 2015, Theorem 3.2). \square

For univariate responses (including binomial ones) under a generalized linear model, a minimally supported design must keep equal weights on all its support points in order to keep D-optimality (Yang and Mandal, 2015). However, for multinomial responses with $J \geq 3$, it is usually not the case. In this section, we use one-predictor ($d = 1$) and two-predictor ($d = 2$) cases for illustration.

In order to check if a minimally supported design is D-optimal, we need a Karush-Kuhn-Tucker-type condition. Since $f(\mathbf{p})$ is log-concave, the Karush-Kuhn-Tucker conditions (Karush, 1939; Kuhn and Tucker, 1951) are also sufficient. We have the following theorem as a direction conclusion.

Theorem 5.10. *An allocation $\mathbf{p} = (p_1^*, \dots, p_m^*)^T$ satisfying $f(\mathbf{p}) > 0$ is D-optimal if and only if there exists a $\lambda \in \mathbb{R}$ such that $\partial f(\mathbf{p})/\partial p_i = \lambda$ if $p_i^* > 0$ or $\leq \lambda$ if $p_i^* = 0$, $i = 1, \dots, m$.*

5.1 Minimally supported designs with one predictor

We first consider the cases with one predictor ($d = 1$). We assume the response has at least three categories ($J \geq 3$) to skip the well-known cases (Example 5.7). The corresponding parameters here are β_1 and $\theta_1, \dots, \theta_{J-1}$.

We start with designs supported on two points ($m = 2$, minimally supported). As a direct conclusion from Theorem 2.2, Lemmas S.4 and S.5, we have:

Theorem 5.11. *Suppose $d = 1$, $J \geq 3$, $m = 2$. The objective function*

$$f(p_1, p_2) = n^{-2} |\mathbf{F}| = \sum_{s=1}^{J-1} c_s p_1^{J-s} p_2^s \quad (5.2)$$

where $(c_1, \dots, c_{J-1})^T = \mathbf{B}_{J-1}^{-1}(d_1, \dots, d_{J-1})^T$ with $\mathbf{B}_{J-1} = (s^{t-1})_{st}$ as a $(J-1) \times (J-1)$ matrix and $d_s = f(1/(s+1), s/(s+1)) \cdot (s+1)^J/s$.

Actually, according to Lemma 2.2, $c_1 = e_2 \prod_{s=1}^{J-1} g_{1s}^2 \cdot \prod_{t=1}^J \pi_{1t}^{-1}(x_1 - x_2)^2$, $c_{J-1} = e_1 \prod_{s=1}^{J-1} g_{2s}^2 \cdot \prod_{t=1}^J \pi_{2t}^{-1}(x_1 - x_2)^2$, where x_1, x_2 are the predictor levels. Theorem 5.11 provides a practically useful way to find out the exact form of

$f(p_1, p_2)$ after calculating $|\mathbf{F}|$ for $J - 1$ different allocations. Then the D-optimal problem is to maximize an order- J polynomial $f(z, 1 - z)$ for $z \in [0, 1]$. As a special case, the D-optimal allocation of $J = 3$ can be solved explicitly as follows:

Corollary 5.2. *Suppose $d = 1$, $J = 3$, $m = 2$. The objective function*

$$f(p_1, p_2) = p_1 p_2 (c_1 p_1 + c_2 p_2) \quad (5.3)$$

where $c_1 = e_2 g_{11}^2 g_{12}^2 (\pi_{11} \pi_{12} \pi_{13})^{-1} (x_1 - x_2)^2 > 0$, $c_2 = e_1 g_{21}^2 g_{22}^2 (\pi_{21} \pi_{22} \pi_{23})^{-1} (x_1 - x_2)^2 > 0$, and x_1, x_2 are the two levels of the predictor. The D-optimal design $\mathbf{p} = (p_1^*, p_2^*)$ is

$$p_1^* = \frac{c_1 - c_2 + \sqrt{c_1^2 - c_1 c_2 + c_2^2}}{2c_1 - c_2 + \sqrt{c_1^2 - c_1 c_2 + c_2^2}}, \quad p_2^* = \frac{c_1}{2c_1 - c_2 + \sqrt{c_1^2 - c_1 c_2 + c_2^2}} \quad (5.4)$$

Furthermore, $p_1^* = p_2^* = 1/2$ if and only if $c_1 = c_2$.

Under the setup of Corollary 5.2, it can be verified that $p_1^* = p_2^* = 1/2$ if $\beta_1 = 0$. In general $p_1^* \neq p_2^*$, and $p_1^* > p_2^*$ if and only if $c_1 > c_2$. The following result provides conditions for D-optimality of such a minimally supported design. Its proof is relegated to the Supplementary Materials (Section S.3).

Corollary 5.3. *Suppose $d = 1$, $J = 3$, $m \geq 3$. Let x_1, \dots, x_m be the m distinct levels of the predictor. A minimally supported design $\mathbf{p} = (p_1^*, p_2^*, 0, \dots, 0)^T$ is D-optimal if and only if*

(1) p_1^*, p_2^* are defined as in (5.4),

(2) $s_{i3}(p_1^*)^2 + (s_{i5} - 2c_1)p_1^* p_2^* + (s_{i4} - c_2)(p_2^*)^2 \leq 0$, $i = 3, \dots, m$,

where c_1, c_2 are same as in Corollary 5.2, $s_{i3} = e_i g_{11}^2 g_{12}^2 (\pi_{11} \pi_{12} \pi_{13})^{-1} (x_1 - x_i)^2 > 0$, $s_{i4} = e_i g_{21}^2 g_{22}^2 (\pi_{21} \pi_{22} \pi_{23})^{-1} (x_2 - x_i)^2 > 0$, $s_{i5} = e_1 (u_{22} u_{i1} + u_{21} u_{i2} - 2b_{22} b_{i2})(x_1 - x_2)(x_1 - x_i) + e_2 (u_{12} u_{i1} + u_{11} u_{i2} - 2b_{12} b_{i2})(x_2 - x_1)(x_2 - x_i) + e_i (u_{12} u_{21} + u_{11} u_{22} - 2b_{12} b_{22})(x_i - x_1)(x_i - x_2)$.

Example 5.8. Suppose $d = 1$, $J = 3$, and $m = 3$ with factor levels $\{-1, 0, 1\}$. Under the logit link g , the parameters $\beta, \theta_1, \theta_2$ satisfy $g(\gamma_{1j}) = \theta_j + \beta$, $g(\gamma_{2j}) = \theta_j$, $g(\gamma_{3j}) = \theta_j - \beta$, $j = 1, 2$. We investigate when a D-optimal design is minimally supported, that is, $p_i = 0$ for some i . According to Theorem 5.11, a D-optimal design satisfies $p_1 = p_3 = 1/2$ if $\beta = 0$. Figure 2 shows cases with more general parameter values. In Figure 2(a), four regions in (θ_1, θ_2) -plane are occupied by minimally supported designs ($\theta_1 < \theta_2$ is required). For example, regions labeled with $p_2 = 0$ indicates a minimally supported design satisfying $p_2 = 0$ is D-optimal given such a triple $(\theta_1, \theta_2, \beta = -2)$. From Figure 2(b), a design supported on $\{-1, 1\}$ (that is, $p_2 = 0$) is D-optimal if β is not far away from 0. \square

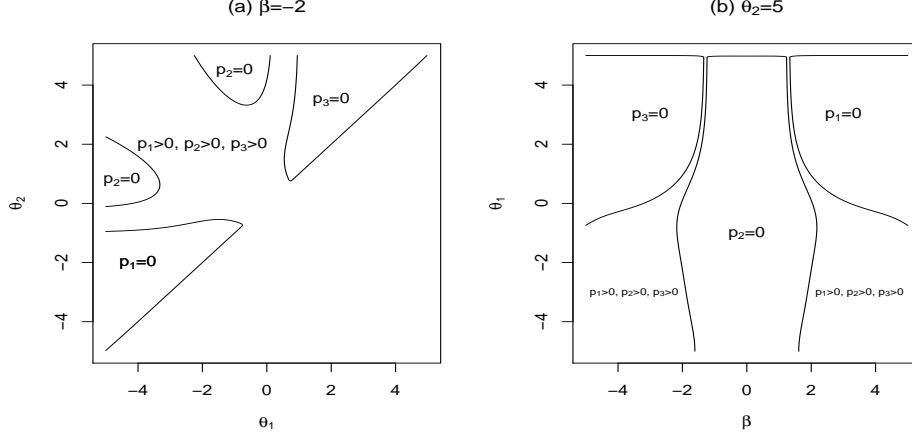


Figure 2: Regions for a two-point design to be D-optimal with $d = 1$, $J = 3$, $x \in \{-1, 0, 1\}$, and logit link (note that $\theta_1 < \theta_2$ is required)

Example 5.9. Toxicity study Agresti (2013, Table 8.7) reported data from a developmental toxicity study with one factor (concentration of diEGdiME at five levels: 0, 62.5, 125, 250, 500 mg/kg per day) and a 3-category ordinal response (status of mouse fetus: **nonlive**, **malformation**, or **normal**). In this case, $d = 1$, $J = 3$, and $m = 5$. For illustration purpose, we fit a cumulative link model with `cauchit` link chosen by both AIC and BIC criteria. The estimated parameter values are $(\hat{\beta}_1, \hat{\theta}_1, \hat{\theta}_2)^T = (-0.0176, -8.80, -5.34)$. Suppose a follow-up experiment is planned with $(\hat{\beta}_1, \hat{\theta}_1, \hat{\theta}_2)^T$ regarded as the true parameter values, then the D-optimal approximate allocation found by the lift-one algorithm is $\mathbf{p}_o = (0, 0, 0, 0.4285, 0.5715)^T$, which is minimally supported. Alternatively, for each pair of indices (i, j) , $1 \leq i < j \leq 5$, we obtain the best design (p_i^*, p_j^*) supported only on x_i, x_j according to Corollary 5.2, then check whether (p_i^*, p_j^*) is D-optimal using Corollary 5.3. We confirm that \mathbf{p}_o is the only minimally supported design that is also D-optimal. With respect to \mathbf{p}_o , the efficiency of the original design (roughly a uniform one) is only 52.6%. \square

5.2 Minimally supported designs with two predictors

In this section, we consider experiments with two predictors ($d = 2$) and a three-category response ($J = 3$). The parameters are $\beta_1, \beta_2, \theta_1, \theta_2$. For cases with $J \geq 4$, similar conclusions could be obtained but with messier notations.

According to Theorem 2.3, a minimally supported design in this case needs three support points, for example, (x_{i1}, x_{i2}) , $i = 1, 2, 3$. Under Assumption 3.3, the 3×3 matrix $\mathbf{X}_1 = (\mathbf{1} \ \mathbf{X})$ is of full rank. Following Theorem 2.2, Lemmas S.4,

S.5, and 2.2, the objective function with $(d, J, m) = (2, 3, 3)$ is

$$f(p_1, p_2, p_3) = |\mathbf{X}_1|^2 e_1 e_2 e_3 \cdot p_1 p_2 p_3 (w_1 p_1 + w_2 p_2 + w_3 p_3) \quad (5.5)$$

where $w_i = e_i^{-1} g_{i1}^2 g_{i2}^2 (\pi_{i1} \pi_{i2} \pi_{i3})^{-1} > 0$. Since $f(p_1, p_2, p_3) = 0$ if $p_1 p_2 p_3 = 0$, we only need to consider $\mathbf{p} = (p_1, p_2, p_3)^T$ satisfying $0 < p_1, p_2, p_3 < 1$.

According to Theorem 5.10, \mathbf{p} maximizes $f(p_1, p_2, p_3)$ only if

$$\frac{\partial f}{\partial p_1} = \frac{\partial f}{\partial p_2} = \frac{\partial f}{\partial p_3} \quad (5.6)$$

Following Tong, Volkmer, and Yang (2014), we obtain its analytic solution:

Theorem 5.12. *Without loss of generality, we assume $w_1 \geq w_2 \geq w_3 > 0$. The allocation $\mathbf{p} = (p_1^*, p_2^*, p_3^*)^T$ maximizing $f(p_1, p_2, p_3)$ in (5.5) exists and is unique. It satisfies $0 < p_3^* \leq p_2^* \leq p_1^* < 1$ and can be obtained analytically as follows*

- (i) *If $w_1 \geq w_2 = w_3$, then $p_1^* = \Delta_1 / (4w_1 + \Delta_1)$, $p_2^* = p_3^* = 2w_1 / (4w_1 + \Delta_1)$, where $\Delta_1 = 2w_1 - 3w_2 + \sqrt{4w_1^2 - 4w_1 w_2 + 9w_2^2}$. A special case is $p_1^* = p_2^* = p_3^* = 1/3$ if $w_1 = w_2 = w_3$.*
- (ii) *If $w_1 = w_2 > w_3$, then $p_1^* = p_2^* = \Delta_2 / [2(\Delta_2 + 2w_1)]$, $p_3^* = 2w_1 / (\Delta_2 + 2w_1)$, where $\Delta_2 = 3w_1 - 2w_3 + \sqrt{9w_1^2 - 4w_1 w_3 + 4w_3^2}$.*
- (iii) *If $w_1 > w_2 > w_3$, then $p_1^* = y_1 / (y_1 + y_2 + 1)$, $p_2^* = y_2 / (y_1 + y_2 + 1)$, $p_3^* = 1 / (y_1 + y_2 + 1)$, where*

$$y_1 = -\frac{b_2}{3} - \frac{2^{1/3}(3b_1 - b_2^2)}{3A^{1/3}} + \frac{A^{1/3}}{3 \times 2^{1/3}}, \quad y_2 = \frac{(w_1 - w_3)y_1}{(w_2 - w_3) + (w_1 - w_2)y_1}$$

with $A = -27b_0 + 9b_1b_2 - 2b_2^3 + 3^{3/2}(27b_0^2 + 4b_1^3 - 18b_0b_1b_2 - b_1^2b_2^2 + 4b_0b_3^2)^{1/2}$, $b_i = c_i/c_3$, $i = 0, 1, 2$, and $c_0 = w_3(w_2 - w_3) > 0$, $c_1 = 3w_1w_2 - w_1w_3 - 4w_2w_3 + 2w_3^2 > 0$, $c_2 = 2w_1^2 - 4w_1w_2 - w_1w_3 + 3w_2w_3$, $c_3 = w_1(w_2 - w_1) < 0$.

The proof of Theorem 5.12 is relegated to the Supplementary Materials (Section S.3). Again, a minimally supported design is usually not uniformly allocated.

Corollary 5.4. *Suppose $d = 2$, $J = 3$, and $m = 3$. Then $\mathbf{p} = (1/3, 1/3, 1/3)^T$ is D -optimal if and only if $w_1 = w_2 = w_3$, where w_1, w_2, w_3 are defined as in (5.5).*

Example 5.10. Consider a typical 2^2 factorial design problem with a three-category response and four design points $(1, 1), (1, -1), (-1, 1), (-1, -1)$, denoted by $(x_{i1}, x_{i2}), i = 1, 2, 3, 4$. That is, $d = 2$, $J = 3$, and $m = 4$. Define $w_i = e_i^{-1} g_{i1}^2 g_{i2}^2 (\pi_{i1} \pi_{i2} \pi_{i3})^{-1}$, $i = 1, 2, 3, 4$. There are five special cases: (i) if $\beta_1 = \beta_2 = 0$, then $w_1 = w_2 = w_3 = w_4$; (ii) if $\beta_1 = 0, \beta_2 \neq 0$, then $w_1 = w_3, w_2 = w_4$, but $w_1 \neq w_2$; (iii) if $\beta_1 \neq 0, \beta_2 = 0$, then $w_1 = w_2, w_3 = w_4$, but $w_1 \neq w_3$; (iv) if $\beta_1 = \beta_2 \neq 0$, then $w_2 = w_3$, but w_1, w_2, w_4 are distinct; (v) if $\beta_1 = -\beta_2 \neq 0$, then $w_1 = w_4$, but w_1, w_2, w_3 are distinct. \square

Theorem 5.12 provides analytic forms of minimally supported designs with $d = 2$ and $J = 3$. As a direct conclusion of Theorem 5.10, we have the necessary and sufficient conditions for D-optimality of a minimally supported design:

Corollary 5.5. *Suppose $d = 2$, $J = 3$, and $m \geq 4$. Let (x_{i1}, x_{i2}) , $i = 1, \dots, m$ be m distinct level combinations of the two predictors. Then $\mathbf{X}_1 = (\mathbf{1} \ \mathbf{X})$ is an $m \times 3$ matrix. A minimally supported design $\mathbf{p} = (p_1^*, p_2^*, p_3^*, 0, \dots, 0)^T$ is D-optimal if and only if (1) p_1^*, p_2^*, p_3^* are obtained according to Theorem 5.12; and (2)*

$$\begin{aligned} & |\mathbf{X}_1[1, 2, i]|^2 e_1 e_2 e_i p_1^* p_2^* (w_1 p_1^* + w_2 p_2^*) + |\mathbf{X}_1[1, 3, i]|^2 e_1 e_3 e_i p_1^* p_3^* (w_1 p_1^* + w_3 p_3^*) \\ & + |\mathbf{X}_1[2, 3, i]|^2 e_2 e_3 e_i p_2^* p_3^* (w_2 p_2^* + w_3 p_3^*) + D_i p_1^* p_2^* p_3^* \\ & \leq |\mathbf{X}_1[1, 2, 3]|^2 e_1 e_2 e_3 p_2^* p_3^* (2w_1 p_1^* + w_2 p_2^* + w_3 p_3^*), \quad \text{for } i = 4, \dots, m, \end{aligned}$$

where $e_j = u_{j1} + u_{j2} - 2b_{j2}$, $w_j = e_j^{-1} g_{j1}^2 g_{j2}^2 (\pi_{j1} \pi_{j2} \pi_{j3})^{-1}$, $j = 1, \dots, m$, $D_i = \sum_{\{j,k,s,t\} \in E_i} e_j e_k (u_{s1} u_{t2} + u_{s2} u_{t1} - 2b_{s2} b_{t2}) \cdot |\mathbf{X}_1[j, k, s]| \cdot |\mathbf{X}_1[j, k, t]|$ with the sum over $E_i = \{(1, 2, 3, i), (1, 3, 2, i), (1, i, 2, 3), (2, 3, 1, i), (2, i, 1, 3), (3, i, 1, 2)\}$.

Example 5.11. Consider experiments with two predictors, a three-category response, and four design points, modeled with logit link. That is, $d = 2$, $J = 3$, $m = 4$. Suppose the four design points are $(1, 1)$, $(1, -1)$, $(-1, 1)$, $(-1, -1)$. According to Theorem 5.12 and Corollary 5.5, we can analytically calculate the best minimally supported design (that is, supported on three points) and determine whether it is D-optimal or not. Figure 3 provides the boundary lines of regions of parameters $(\beta_1, \beta_2, \theta_1, \theta_2)$ for which the best three-point design is D-optimal. In particular, Figure 3(a) shows the region of (β_1, β_2) for given θ_1, θ_2 . It clearly indicates that the best three-point design tends to be D-optimal when the absolute values of β_1, β_2 are large. The region tends to be larger as the absolute values of θ_1, θ_2 increase. On the other hand, Figure 3(b) displays the region of (θ_1, θ_2) for given β_1, β_2 . The symmetry of the boundary lines about $\theta_1 + \theta_2 = 0$ is due to the logit link which is symmetric about 0. An interesting conclusion based on Corollary 5.5 is that in this case a three-point design can never be D-optimal if $\beta_1 = 0$ or $\beta_2 = 0$. \square

Remark 5.1. In this section we show that the extra degrees of freedom plays an important role against the uniformity of D-optimal allocation in a minimally supported design. For multinomial-type responses with J categories, the total degrees of freedom from m distinct experimental settings is $m(J - 1)$, while a cumulative link model contains $d + J - 1$ parameters. For a minimally supported design, $m = d + 1$ and $m(J - 1) = d + J - 1$ if and only if $J = 2$ (see Example 5.7). In that case, the objective function $f(\mathbf{p}) \propto p_{i_0} p_{i_1} \cdots p_{i_d}$ and thus the D-optimal allocation is $p_{i_0} = p_{i_1} = \cdots = p_{i_d} = 1/(d + 1)$. However, if $J \geq 3$, then the degrees

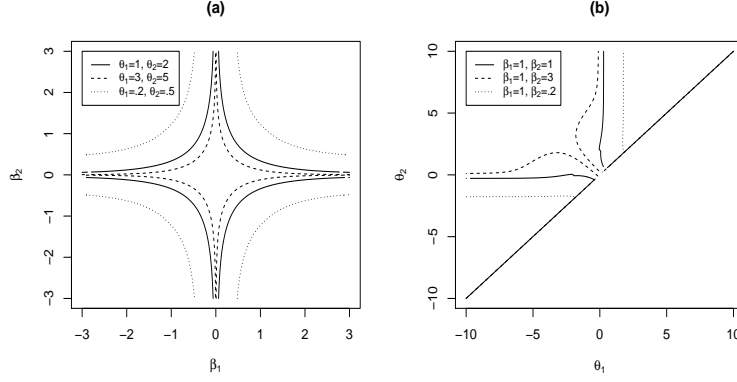


Figure 3: Boundary lines for a three-point design to be D-optimal with logit link: Region of (β_1, β_2) for given (θ_1, θ_2) is outside the boundary lines in Panel (a); Region of (θ_1, θ_2) (with $\theta_1 < \theta_2$) for given (β_1, β_2) is between the boundary lines and $\theta_1 = \theta_2$ in Panel (b)

of freedom is strictly bigger than the number of parameters and there are “extra” degrees of freedom. In this case, distinct experimental settings may play different roles in estimating the parameters values. For example, if $d = 1, J = 3, m = 2$, the objective function $f(\mathbf{p}) = p_1 p_2 (c_1 p_1 + c_2 p_2)$ according to Corollary 5.2; if $d = 2, J = 3, m = 3$, $f(\mathbf{p}) \propto p_1 p_2 p_3 (w_1 p_1 + w_2 p_2 + w_3 p_3)$ according to equation (5.5). In those cases, the D-optimality of a uniform allocation depends on $c_1 = c_2$ or $w_1 = w_2 = w_3$, which is not true in general.

6. EW D-optimal Design

The previous sections mainly focus on locally D-optimal designs which require assumed parameter values, $(\beta_1, \dots, \beta_d, \theta_1, \dots, \theta_{J-1})$. For many applications, the experimenter may have little or limited information about the values of parameters. In that case, Bayes D-optimality (Chaloner and Verdinelli, 1995) which maximizes $E(\log |\mathbf{F}|)$ given a prior distribution on parameters provides a reasonable solution. An alternative to Bayes one is the EW D-optimality (Yang, Mandal, and Majumdar, 2016; Atkinson et al., 2007) which maximizes $\log |E(\mathbf{F})|$ essentially. According to Yang, Mandal, and Majumdar (2016)’s thorough simulation study across different models and choices of priors, EW D-optimal designs are much easier to calculate and still highly efficient compared with Bayes ones.

Based on Theorem 2.1, an EW D-optimal design which maximizes $|E(\mathbf{F})|$ may be viewed as a locally D-optimal design with e_i, c_{it}, u_{it} and b_{it} replaced by their expectations. After the replacement, Lemma S.2 still holds. Therefore, almost all the lemmas, theorems, corollaries, and algorithms in the previous sections can be applied directly to EW D-optimal designs as well. The only

exception is due to Lemma 2.1 which provides the formula of $|\mathbf{A}_{i3}|$ in terms of g_{ij} and π_{ij} . In order to fit EW D-optimal designs, $|\mathbf{A}_{i3}|$ needs to be calculated in terms of u_{it} and b_{it} . For example, $|\mathbf{A}_{i3}| = u_{i1}$ if $J = 2$, $|\mathbf{A}_{i3}| = u_{i1}u_{i2} - b_{i2}^2$ if $J = 3$, and $|\mathbf{A}_{i3}| = u_{i1}u_{i2}u_{i3} - u_{i1}b_{i3}^2 - u_{i3}b_{i2}^2$ if $J = 4$. Then the formulas of $|\mathbf{A}_{i3}|$ in Lemma 2.2, c_1, c_2 in Corollary 5.2, s_{i3}, s_{i4}, s_{i5} in Corollary 5.3, w_i in (5.5), and w_j in Corollary 5.5 need to be written in terms of u_{it} and b_{it} as well.

According to Lemma S.2, we only need to calculate $E(u_{it}), i = 1, \dots, m; t = 1, \dots, J-1$ and $E(b_{it}), i = 1, \dots, m; t = 2, \dots, J-1$ (if $J \geq 3$). Then $E(c_{it}) = E(u_{it}) - E(b_{it}) - E(b_{i,t+1})$ and $E(e_i) = \sum_{t=1}^{J-1} E(c_{it})$. After that, we can use the lift-one algorithm in Section 3 or the exchange algorithm in Section 4 to find EW D-optimal designs. We use the odor removal example to illustrate how it works.

Example 3.4 : Odor Removal Study (*continued*) Again suppose that we plan to conduct a followup experiment. Instead of assuming the parameter values $(\beta_1, \beta_2, \theta_1, \theta_2) = (-2.44, 1.09, -2.67, -0.21)$, suppose we believe that the true values of parameters satisfy $\beta_1 \in [-3, -1]$, $\beta_2 \in [0, 2]$, $\theta_1 \in [-4, -2]$, and $\theta_2 \in [-1, 1]$. In order to perform Bayes optimality, we assume that the four parameters are independently and uniformly distributed within their intervals. We use R function `constrOptim` to maximize $\phi(\mathbf{p}) = E(\log |\mathbf{F}|)$ and find the Bayes D-optimal allocation $\mathbf{p}_b = (0.3879, 0.3264, 0.0000, 0.2857)^T$. The procedure costs 313 seconds computational time. In order to get the EW D-optimal design, we only need 5.43 seconds in total to calculate $E(u_{it})$ and $E(b_{it})$ and find $\mathbf{p}_e = (0.3935, 0.3259, 0, 0.2806)^T$ using the lift-one algorithm. Even in terms of Bayes Optimality (Chaloner and Larntz, 1989; Song and Wong, 1998; Abebe et al., 2014), the relative efficiency of \mathbf{p}_e with respect to \mathbf{p}_b is $\exp\{(\phi(\mathbf{p}_e) - \phi(\mathbf{p}_b))/4\} \times 100\% = 99.99\%$, while the relative efficiency of the uniform allocation $\mathbf{p}_u = (0.25, 0.25, 0.25, 0.25)^T$ is only 87.67%.

In order to check *robustness* towards misspecified parameter values, we let $\boldsymbol{\theta} = (\beta_1, \beta_2, \theta_1, \theta_2)^T$ run through all 0.1-grid points in $[-3, -1] \times [0, 2] \times [-4, -2] \times [-1, 1]$, that is, the set of $\mathbf{I} = \{-3, -2.9, \dots, -1\} \times \{0, 0.1, \dots, 2\} \times \{-4, -3.9, \dots, -2\} \times \{-1, -0.9, \dots, 1\}$. For each $\boldsymbol{\theta} \in \mathbf{I}$, we use the lift-one algorithm to find the D-optimal allocation $\mathbf{p}_{\boldsymbol{\theta}}$ and the corresponding determinant $f(\mathbf{p}_{\boldsymbol{\theta}}) = |\mathbf{F}(\mathbf{p}_{\boldsymbol{\theta}})|$, and then calculate the efficiency $(f(\mathbf{p})/f(\mathbf{p}_{\boldsymbol{\theta}}))^{1/4}$ for $\mathbf{p} = \mathbf{p}_b, \mathbf{p}_e$, and \mathbf{p}_u , respectively. Table 3 shows the summary statistics of the efficiencies for $\boldsymbol{\theta} \in \mathbf{I}$. It implies that \mathbf{p}_b and \mathbf{p}_e are comparable and both of them are much better than \mathbf{p}_u in terms of robustness. \square

7. Discussion

In this paper, we use four real experiments to illustrate how much improvements the experimenter could make by adopting our D-optimal designs, including Example 3.4: Odor removal study; Example 3.5: Wine bitterness study; Example 4.6: Polysilicon deposition study; and Example 5.9: Toxicity study. In the

Table 3: Summary of Efficiency in Odor Removal Study

Design	Min.	1st Quartile	Median	Mean	3rd Quartile	Max.
Bayes \mathbf{p}_b	0.8464	0.9813	0.9915	0.9839	0.9964	1.0000
EW \mathbf{p}_e	0.8465	0.9802	0.9917	0.9838	0.9967	1.0000
Uniform \mathbf{p}_u	0.7423	0.8105	0.8622	0.8674	0.9249	0.9950

absence of theoretical results on optimal designs for ordinal data, their original designs are either uniform designs with equal number of replicates or regular fractional designs (Example 4.6) following the classical results under linear models. Although these original designs are common in practice, their efficiencies compared with our D-optimal designs are often far from satisfactory: 79.7% in Example 3.4, 73.1% in Example 4.6, and 52.6% in Example 5.9.

More interestingly, our D-optimal designs recommended for Example 3.4 and Example 5.9 are both minimally supported, that is, these designs require the minimum number of experimental settings, which indicates the minimum cost and minimum time spent for running the experiments (Phadke, 1989). We have two surprising findings that are different from the cases under univariate generalized linear models (Yang and Mandal, 2015): (1) the minimum number of experimental settings can be strictly less than the number of parameters: 3 experimental settings for 4 parameters in Example 3.4, and 2 experimental settings for 3 parameters in Example 5.9; (2) the allocation of experimental units on the support points of a minimally supported design is usually not uniform: $(p_1, p_2, p_4) = (0.4449, 0.2871, 0.2680)$ in Example 3.4, and $(p_4, p_5) = (0.4285, 0.5715)$ in Example 5.9. These findings have been justified theoretically. The apparent anomaly is explained by the fact that a single experimental setting or support point with multiple-category responses generates more than one independent summary statistics, and thus produces enough degrees of freedom to estimate more parameters than the number of experimental settings.

Even when the experimenter has little information about the parameters, we recommend the use of EW D-optimal designs instead of uniform designs. It is easy to obtain them using our algorithms and they are much more robust than uniform designs, which is illustrated using Example 3.4. The EW D-optimal designs are highly efficient surrogate to Bayesian D-optimal designs as well.

Cumulative link models are widely used for modeling ordinal data. Nevertheless, there are other models used for multinomial-type responses, including baseline-category logit model for nominal response, adjacent-categories logit model for ordinal data, and continuation-ratio logit model for hierarchical response (see Liu and Agresti (2005), Agresti (2013) for a review). The methods developed in this paper could be extended for those models as well. For further

extension, our approaches could be used for planning experiments with more than one categorical responses. For example, both the paper feeder experiment and the PCB experiment analyzed by Joseph and Wu (2004) involved multiple binomial responses. The characteristics of optimal designs for these experiments are expected to be different from the ones with univariate responses as well.

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D-OPTIMAL DESIGNS WITH ORDERED CATEGORICAL DATA

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Supplementary Materials

S.1 Commonly Used Link Functions for Cumulative Link Models

Link function	$g(\gamma)$	$g^{-1}(\eta)$	$(g^{-1})'(\eta)$
logit	$\log\left(\frac{\gamma}{1-\gamma}\right)$	$\frac{e^\eta}{1+e^\eta}$	$\frac{e^\eta}{(1+e^\eta)^2}$
probit	$\Phi^{-1}(\gamma)$	$\Phi(\eta)$	$\phi(\eta)$
log-log	$-\log[-\log(\gamma)]$	$\exp\{-e^{-\eta}\}$	$\exp\{-\eta - e^{-\eta}\}$
complementary log-log	$\log[-\log(1-\gamma)]$	$1 - \exp\{-e^\eta\}$	$\exp\{\eta - e^\eta\}$
cauchit	$\tan[\pi(\gamma - \frac{1}{2})]$	$\frac{1}{\pi} \arctan(\eta) + \frac{1}{2}$	$\frac{1}{\pi(1+\eta^2)}$

where $\Phi^{-1}(\cdot)$ is the cumulative distribution function of $N(0, 1)$, and $\phi(\cdot)$ is the probability density function of $N(0, 1)$.

Example 2.1 (*continued*) For logit link g , $g^{-1}(\eta) = e^\eta / (1 + e^\eta)$ and $(g^{-1})' = g^{-1}(1 - g^{-1})$. Thus $g_{ij} = (g^{-1})'(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta}) = (\gamma_{ij})(1 - \gamma_{ij})$. With $J = 3$, we have $\pi_{i1} + \pi_{i2} + \pi_{i3} = 1$ for $i = 1, \dots, m$. Then for $i = 1, \dots, m$, $g_{i1} = \pi_{i1}(\pi_{i2} + \pi_{i3})$, $g_{i2} = (\pi_{i1} + \pi_{i2})\pi_{i3}$, $b_{i2} = \pi_{i1}\pi_{i3}\pi_{i2}^{-1}(\pi_{i1} + \pi_{i2})(\pi_{i2} + \pi_{i3})$, $u_{i1} = \pi_{i1}\pi_{i2}^{-1}(\pi_{i1} + \pi_{i2})(\pi_{i2} + \pi_{i3})^2$, $u_{i2} = \pi_{i3}\pi_{i2}^{-1}(\pi_{i1} + \pi_{i2})^2(\pi_{i2} + \pi_{i3})$, $c_{i1} = \pi_{i1}(\pi_{i1} + \pi_{i2})(\pi_{i2} + \pi_{i3})$, $c_{i2} = \pi_{i3}(\pi_{i1} + \pi_{i2})(\pi_{i2} + \pi_{i3})$, $e_i = (\pi_{i1} + \pi_{i2})(\pi_{i1} + \pi_{i3})(\pi_{i2} + \pi_{i3})$

□

S.2 Additional Lemmas

For Section 2: Since $(Y_{i1}, \dots, Y_{iJ}), i = 1, \dots, m$ are independent, the log-likelihood function (up to a constant) of the cumulative link model is

$$l(\beta_1, \dots, \beta_d, \theta_1, \dots, \theta_{J-1}) = \sum_{i=1}^m \sum_{j=1}^J Y_{ij} \log(\pi_{ij})$$

where $\pi_{ij} = \gamma_{ij} - \gamma_{i,j-1}$ with $\gamma_{ij} = g^{-1}(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta})$ for $j = 1, \dots, J-1$ and $\gamma_{i0} = 0$, $\gamma_{iJ} = 1$, $i = 1, \dots, m$. For $s = 1, \dots, d$, $t = 1, \dots, J-1$,

$$\begin{aligned} \frac{\partial l}{\partial \beta_s} &= \sum_{i=1}^m (-x_{is}) \cdot \left\{ \frac{Y_{i1}}{\pi_{i1}} \cdot (g^{-1})'(\theta_1 - \mathbf{x}_i^T \boldsymbol{\beta}) \right. \\ &\quad + \frac{Y_{i2}}{\pi_{i2}} \cdot [(g^{-1})'(\theta_2 - \mathbf{x}_i^T \boldsymbol{\beta}) - (g^{-1})'(\theta_1 - \mathbf{x}_i^T \boldsymbol{\beta})] \\ &\quad \left. + \dots + \frac{Y_{iJ}}{\pi_{iJ}} [-(g^{-1})'(\theta_{J-1} - \mathbf{x}_i^T \boldsymbol{\beta})] \right\} \\ \frac{\partial l}{\partial \theta_t} &= \sum_{i=1}^m (g^{-1})'(\theta_t - \mathbf{x}_i^T \boldsymbol{\beta}) \left(\frac{Y_{it}}{\pi_{it}} - \frac{Y_{i,t+1}}{\pi_{i,t+1}} \right) \end{aligned}$$

Since Y_{ij} 's come from multinomial distributions, we know $E(Y_{ij}) = n_i \pi_{ij}$, $E(Y_{ij}^2) = n_i(n_i - 1)\pi_{ij}^2 + n_i \pi_{ij}$, and $E(Y_{is}Y_{it}) = n_i(n_i - 1)\pi_{is}\pi_{it}$ when $s \neq t$. Then we have the following lemma:

Lemma S.1. *Let $\mathbf{F} = (F_{st})$ be the $(d + J - 1) \times (d + J - 1)$ Fisher information matrix.*

(i) *For $1 \leq s \leq d$, $1 \leq t \leq d$,*

$$\mathbf{F}_{st} = E \left(\frac{\partial l}{\partial \beta_s} \frac{\partial l}{\partial \beta_t} \right) = \sum_{i=1}^m n_i x_{is} x_{it} \sum_{j=1}^J \frac{(g_{ij} - g_{i,j-1})^2}{\pi_{ij}}$$

where $g_{ij} = (g^{-1})'(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta}) > 0$ for $j = 1, \dots, J-1$ and $g_{i0} = g_{iJ} = 0$.

(ii) *For $1 \leq s \leq d$, $1 \leq t \leq J-1$,*

$$F_{s,d+t} = E \left(\frac{\partial l}{\partial \beta_s} \frac{\partial l}{\partial \theta_t} \right) = \sum_{i=1}^m n_i (-x_{is}) g_{it} \left(\frac{g_{it} - g_{i,t-1}}{\pi_{it}} - \frac{g_{i,t+1} - g_{it}}{\pi_{i,t+1}} \right)$$

(iii) *For $1 \leq s \leq J-1$, $1 \leq t \leq d$,*

$$F_{d+s,t} = E \left(\frac{\partial l}{\partial \theta_s} \frac{\partial l}{\partial \beta_t} \right) = \sum_{i=1}^m n_i (-x_{it}) g_{is} \left(\frac{g_{is} - g_{i,s-1}}{\pi_{is}} - \frac{g_{i,s+1} - g_{is}}{\pi_{i,s+1}} \right)$$

(iv) For $1 \leq s \leq J-1, 1 \leq t \leq J-1$,

$$F_{d+s,d+t} = E \left(\frac{\partial l}{\partial \theta_s} \frac{\partial l}{\partial \theta_t} \right) = \begin{cases} \sum_{i=1}^m n_i g_{is}^2 (\pi_{is}^{-1} + \pi_{i,s+1}^{-1}), & \text{if } s = t \\ \sum_{i=1}^m n_i g_{is} g_{it} (-\pi_{i,s \vee t}^{-1}), & \text{if } |s - t| = 1 \\ 0, & \text{if } |s - t| \geq 2 \end{cases}$$

where $s \vee t = \max\{s, t\}$.

Perevozskaya et al. (2003) obtained a detailed form of Fisher information matrix for logit link and one predictor. Our expressions here are good for fairly general link and d predictors. To simplify the notations, we denote

$$e_i = \sum_{j=1}^J \frac{(g_{ij} - g_{i,j-1})^2}{\pi_{ij}} > 0, \quad i = 1, \dots, m \quad (\text{S.1})$$

$$c_{it} = g_{it} \left(\frac{g_{it} - g_{i,t-1}}{\pi_{it}} - \frac{g_{i,t+1} - g_{it}}{\pi_{i,t+1}} \right), i = 1, \dots, m; t = 1, \dots, J-1 \quad (\text{S.2})$$

$$u_{it} = g_{it}^2 (\pi_{it}^{-1} + \pi_{i,t+1}^{-1}) > 0, \quad i = 1, \dots, m; t = 1, \dots, J-1 \quad (\text{S.3})$$

$$b_{it} = g_{i,t-1} g_{it} \pi_{it}^{-1} > 0, \quad i = 1, \dots, m; t = 2, \dots, J-1 \text{ (if } J \geq 3) \quad (\text{S.4})$$

Note that g_{ij} is defined in Lemma S.1 (i). Then we obtain the following lemma which plays a key role in later on calculation of $|\mathbf{F}|$.

Lemma S.2. $c_{it} = u_{it} - b_{it} - b_{i,t+1}$, $i = 1, \dots, m; t = 1, \dots, J-1$; $e_i = \sum_{t=1}^{J-1} c_{it} = \sum_{t=1}^{J-1} (u_{it} - 2b_{it})$, $i = 1, \dots, m$, where $b_{i1} = b_{iJ} = 0$ for $i = 1, \dots, m$.

Lemma S.3. $\text{Rank}((\mathbf{A}_{i1} \mathbf{A}_{i2})) \leq 1$ where “=” is true if and only if $\mathbf{x}_i \neq 0$.

Based on Lemma 2.1 and Lemma S.3, we can obtain the two lemmas below on $c_{\alpha_1, \dots, \alpha_m}$ which significantly simplify the structure of $|\mathbf{F}|$ as a polynomial of (n_1, \dots, n_m) .

Lemma S.4. If $\max_{1 \leq i \leq m} \alpha_i \geq J$, then $|\mathbf{A}_\tau| = 0$ for any $\tau \in (\alpha_1, \dots, \alpha_m)$ and thus $c_{\alpha_1, \dots, \alpha_m} = 0$.

Proof of Lemma S.4: Without any loss of generality, we assume $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_m$. Then $\max_{1 \leq i \leq m} \alpha_i \geq J$ implies $\alpha_1 \geq J$. In this case, for any $\tau \in (\alpha_1, \dots, \alpha_m)$, $\tau^{-1}(1) := \{i \mid \tau(i) = 1\} \subset \{1, \dots, d+J-1\}$ and $|\tau^{-1}(1)| = \alpha_1$. If $|\tau^{-1}(1) \cap \{1, \dots, d\}| \geq 2$, then $|\mathbf{A}_\tau| = 0$ due to Lemma S.3; otherwise

$\{d+1, \dots, d+J-1\} \subset \tau^{-1}(1)$ and thus $|A_\tau| = 0$ due to Lemma 2.1. Thus $c_{\alpha_1, \dots, \alpha_m} = 0$ according to (2.3) provided in Theorem 2.2. \square

Lemma S.5. *If $\#\{i : \alpha_i \geq 1\} \leq d$, then $|A_\tau| = 0$ for any $\tau \in (\alpha_1, \dots, \alpha_m)$ and thus $c_{\alpha_1, \dots, \alpha_m} = 0$.*

Proof of Lemma S.5: Without any loss of generality, we assume $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_m$. Then $\#\{i : \alpha_i \geq 1\} \leq d$ indicates $\alpha_{d+1} = \dots = \alpha_m = 0$. Let $\tau : \{1, 2, \dots, d+J-1\} \rightarrow \{1, \dots, m\}$ satisfy $\tau \in (\alpha_1, \dots, \alpha_m)$. Then the $(d+J-1) \times (d+J-1)$ matrix A_τ can be written as

$$\begin{pmatrix} A_{\tau 1} & A_{\tau 2} \\ A_{\tau 3} & A_{\tau 4} \end{pmatrix} = \begin{pmatrix} (e_{\tau(s)} x_{\tau(s)s} x_{\tau(s)t})_{s=1, \dots, d; t=1, \dots, d} & (-x_{\tau(s)s} c_{\tau(s)t})_{s=1, \dots, d; t=1, \dots, J-1} \\ (-c_{\tau(d+s)s} x_{\tau(d+s)t})_{s=1, \dots, J-1; t=1, \dots, d} & A_{\tau 4} \end{pmatrix}$$

where the $(J-1) \times (J-1)$ matrix $A_{\tau 4}$ is either a single entry $u_{\tau(d+1)1}$ (if $J = 2$) or symmetric tri-diagonal with diagonal entries $u_{\tau(d+1)1}, \dots, u_{\tau(d+J-1), J-1}$, upper off-diagonal entries $-b_{\tau(d+1)2}, \dots, -b_{\tau(d+J-2), J-1}$, and lower off-diagonal entries $-b_{\tau(d+2)2}, \dots, -b_{\tau(d+J-1), J-1}$. Note that A_τ is asymmetric in general.

If $\#\{i : \alpha_i \geq 1\} \leq d-1$, then there exists an i_0 such that $1 \leq i_0 \leq d$ and $|\tau^{-1}(i_0) \cap \{1, \dots, d\}| \geq 2$. In this case, $|A_\tau| = 0$ according to Lemma S.3.

If $\#\{i : \alpha_i \geq 1\} = d$, we may assume $|\tau^{-1}(i) \cap \{1, \dots, d\}| = 1$ for $i = 1, \dots, d$ (otherwise $|A_\tau| = 0$ according to Lemma S.3). Suppose $\alpha_1 \geq \alpha_2 \geq \dots \geq \alpha_k \geq 2 > \alpha_{k+1}$. Then $\{d+1, \dots, d+J-1\} \subset \cup_{i=1}^k \tau^{-1}(i)$ and $\sum_{i=1}^k (\alpha_i - 1) = J-1$. In order to show $|A_\tau| = 0$, we first replace $A_{\tau 1}$ with $A_{\tau 1}^{(1)} = (e_{\tau(s)} x_{\tau(s)s})_{s=1, \dots, d; t=1, \dots, d}$ and replace $A_{\tau 2}$ with $A_{\tau 2}^{(1)} = (-c_{\tau(s)t})_{s=1, \dots, d; t=1, \dots, J-1}$. It changes A_τ into a new matrix $A_\tau^{(1)}$. Note that $|A_\tau| = \prod_{s=1}^d x_{\tau(s)s} \cdot |A_\tau^{(1)}|$. According to Lemma S.2, the sum of the columns of $A_{\tau 2}^{(1)}$ is $(-e_{\tau(1)}, \dots, -e_{\tau(d)})^T$, and the elementwise sum of the columns of $A_{\tau 4}$ is $(c_{\tau(d+1)1}, c_{\tau(d+2)2}, \dots, c_{\tau(d+J-1), J-1})^T$. Secondly, for $t = 1, \dots, d$, we add $x_{1t}(-e_{\tau(1)}, \dots, -e_{\tau(d)}, c_{\tau(d+1)1}, \dots, c_{\tau(d+J-1), J-1})^T$ to the t th column of $A_\tau^{(1)}$. We denote the resulting matrix by $A_\tau^{(2)}$. Note that $|A_\tau^{(1)}| = |A_\tau^{(2)}|$. We consider the sub-matrix $A_{\tau d}^{(2)}$ which consists of the first d columns of $A_\tau^{(2)}$. For $s \in \tau^{-1}(1)$, the s th row of $A_{\tau d}^{(2)}$ is simply 0. For $i = 2, \dots, k$, the j th row of $A_{\tau d}^{(2)}$ is proportional to $(x_{i1} - x_{11}, x_{i2} - x_{12}, \dots, x_{id} - x_{1d})$ if $j \in \tau^{-1}(i)$.

Therefore, $\text{Rank}(A_{\tau d}^{(2)}) \leq (d + J - 1) - \alpha_1 - \sum_{i=2}^k (\alpha_i - 1) = d - 1$, which leads to $|A_{\tau}^{(2)}| = 0$ and thus $|A_{\tau}^{(1)}| = 0$, $|A_{\tau}| = 0$. According to (2.3) in Theorem 2.2, $c_{\alpha_1, \dots, \alpha_m} = 0$. \square

Lemma S.6. $\mathbf{F} = \mathbf{F}(\mathbf{p})$ is always positive semi-definite. It is positive definite if and only if $\mathbf{p} \in S_+$. Furthermore, $\log f(\mathbf{p})$ is concave on S .

For Section 5.2: The procedure seeking for analytic solutions here follows Tong, Volkmer, and Yang (2014). As a direct conclusion of the Karush-Kuhn-Tucker conditions (see also Theorem 5.10), a necessary condition for (p_1, p_2, p_3) to maximize $f(p_1, p_2, p_3)$ in (5.5) is (5.6), which are equivalent to $\partial f / \partial p_1 = \partial f / \partial p_3$, $\partial f / \partial p_2 = \partial f / \partial p_3$. In terms of p_i, w_i 's, they are

$$(p_3 - p_1)(p_1 w_1 + p_2 w_2 + p_3 w_3) = (w_3 - w_1)p_1 p_3 \quad (\text{S.5})$$

$$(p_3 - p_2)(p_1 w_1 + p_2 w_2 + p_3 w_3) = (w_3 - w_2)p_2 p_3 \quad (\text{S.6})$$

Denote $y_1 = p_1/p_3 > 0$ and $y_2 = p_2/p_3 > 0$. Since $p_1 + p_2 + p_3 = 1$, it implies $p_3 = 1/(y_1 + y_2 + 1)$, $p_1 = y_1/(y_1 + y_2 + 1)$, and $p_2 = y_2/(y_1 + y_2 + 1)$. In terms of y_1, y_2 , (S.5) and (S.6) are equivalent to

$$(1 - y_1)(y_1 w_1 + y_2 w_2 + w_3) = (w_3 - w_1)y_1 \quad (\text{S.7})$$

$$(1 - y_2)(y_1 w_1 + y_2 w_2 + w_3) = (w_3 - w_2)y_2 \quad (\text{S.8})$$

Lemma S.7. Suppose $0 < w_3 < w_2 < w_1$. If (p_1, p_2, p_3) maximizes $f(p_1, p_2, p_3)$ in (5.5) under the constraints $p_1, p_2, p_3 \geq 0$ and $p_1 + p_2 + p_3 = 1$, then $0 < p_3 \leq p_2 \leq p_1 < 1$.

The proof of the lemma above is straightforward. Because otherwise one could exchange p_i, p_j to strictly improve $f(p_1, p_2, p_3)$. Now we are ready to get solutions to equations (S.7) and (S.8) case by case.

- (i) $w_1 = w_3$. In that case, (S.7) implies $y_1 = 1$. After plugging it into (S.8), the only positive solution is $y_2 = (-3w_1 + 2w_2 + \sqrt{9w_1^2 - 4w_1 w_2 + 4w_2^2})/(2w_2)$.
- (ii) $w_2 = w_3$. In that case, (S.8) implies $y_2 = 1$. After plugging it into (S.7), the only positive solution is $y_1 = (2w_1 - 3w_2 + \sqrt{4w_1^2 - 4w_1 w_2 + 9w_2^2})/(2w_1)$.

- (iii) $w_1 = w_2$ but $w_1 \neq w_3$ and $w_2 \neq w_3$. The ratio of (S.7) and (S.8) leads to $y_1 = y_2$. After plugging it into (S.7), the only positive solution is $y_1 = (3w_1 - 2w_3 + \sqrt{9w_1^2 - 4w_1w_3 + 4w_3^2})/(4w_1)$.
- (iv) w_1, w_2, w_3 are distinct. Without any loss of generality, we assume $0 < w_3 < w_2 < w_1$. (Otherwise the previous elimination procedure in the order of p_3, p_2, p_1 could be easily changed accordingly.) Based on Lemma S.7, if (p_1, p_2, p_3) maximizes f_4 , then $0 < p_3 \leq p_2 \leq p_1 < 1$ and thus $y_1 \geq y_2 \geq 1$. The ratio of (S.7) and (S.8) leads to $(1 - y_1)/(1 - y_2) = (w_3 - w_1)/(w_3 - w_2) \cdot y_1/y_2$, which implies

$$y_2 = \frac{(w_1 - w_3)y_1}{(w_2 - w_3) + (w_1 - w_2)y_1}. \quad (\text{S.9})$$

Note that $(w_2 - w_3) + (w_1 - w_2)y_1 \geq w_1 - w_3 > 0$. After plugging (S.9) into (S.7), we get

$$c_0 + c_1y_1 + c_2y_1^2 + c_3y_1^3 = 0 \quad (\text{S.10})$$

where $c_0 = w_3(w_2 - w_3) > 0$, $c_1 = 3w_1w_2 - w_1w_3 - 4w_2w_3 + 2w_3^2 > 0$, $c_2 = 2w_1^2 - 4w_1w_2 - w_1w_3 + 3w_2w_3$, $c_3 = w_1(w_2 - w_1) < 0$.

Lemma S.8. *Suppose $0 < w_3 < w_2 < w_1$. Then equation (S.10) has one and only one solution $y_1^* \geq 1$. Furthermore, $y_1^* > 1$.*

Proof of Lemma S.8: In order to locate the roots of equation (S.10), we let $f_1(y_1) = c_0 + c_1y_1 + c_2y_1^2 + c_3y_1^3$. Then $f_1(1) = c_0 + c_1 + c_2 + c_3 = (w_1 - w_3)^2 > 0$.

On the other hand, the first derivative of f_1 is $f_1'(y_1) = a_0 + a_1y_1 + a_2y_1^2$, where $a_0 = 3w_1w_2 - w_1w_3 - 4w_2w_3 + 2w_3^2 = w_1(w_2 - w_3) + 2(w_1 - w_2)w_2 + 2(w_2 - w_3)^2 > 0$, $a_1 = 2(2w_1^2 - 4w_1w_2 - w_1w_3 + 3w_2w_3)$, and $a_2 = 3w_1(w_2 - w_1) < 0$. Therefore, $a_1^2 - 4a_0a_2 > a_1^2 \geq 0$ and $f_1'(y_1) = a_2(y_1 - y_{11})(y_1 - y_{12})$, where

$$y_{11} = \frac{-a_1 + \sqrt{a_1^2 - 4a_0a_2}}{2a_2} < 0, \quad y_{12} = \frac{-a_1 - \sqrt{a_1^2 - 4a_0a_2}}{2a_2} > y_{11}$$

It can be verified that $y_{12} < 1$ if and only if $w_1 < 2(w_2 + w_3)$. There are two cases: *Case (i):* If $y_{12} < 1$, then $f_1'(y_1) < 0$ for all $y_1 > 1$. That is, $f_1(y_1)$ strictly decreases after $y_1 = 1$. Since $f_1(1) > 0$ and $f_1(\infty) = -\infty$, then there is one and only one solution in $(1, \infty)$; *Case (ii):* If $y_{12} \geq 1$, then $f_1'(y_1) \geq 0$ for $y_1 \in [1, y_{12}]$

and $f_1'(y_1) < 0$ for $y_1 \in (y_{12}, \infty)$. That is, $f_1(y_1)$ increases in $[1, y_{12}]$ and then strictly decreases in (y_{12}, ∞) . Again, due to $f_1(1) > 0$ and $f_1(\infty) = -\infty$, there is one and only one solution in $(1, \infty)$. In either case, the conclusion is justified. \square

S.3 Additional Proofs

Proof of Theorem 2.1 As a direct conclusion of Lemma S.1 and Lemma S.2, we obtain Theorem 2.1. \square

Examples of \mathbf{A}_{i3} in Theorem 2.1 include (u_{i1}) ,

$$\begin{pmatrix} u_{i1} & -b_{i2} \\ -b_{i2} & u_{i2} \end{pmatrix}, \begin{pmatrix} u_{i1} & -b_{i2} & 0 \\ -b_{i2} & u_{i2} & -b_{i3} \\ 0 & -b_{i3} & u_{i3} \end{pmatrix}, \begin{pmatrix} u_{i1} & -b_{i2} & 0 & 0 \\ -b_{i2} & u_{i2} & -b_{i3} & 0 \\ 0 & -b_{i3} & u_{i3} & -b_{i4} \\ 0 & 0 & -b_{i4} & u_{i4} \end{pmatrix}$$

for $J = 2, 3, 4$, or 5 respectively.

Proof of Theorem 2.2 To study the structure of $|\mathbf{F}|$ as a polynomial function of (n_1, \dots, n_m) , we denote the (k, l) th entry of \mathbf{A}_i by $a_{kl}^{(i)}$. Given a row map $\tau : \{1, 2, \dots, d+J-1\} \rightarrow \{1, \dots, m\}$, we define a $(d+J-1) \times (d+J-1)$ matrix $\mathbf{A}_\tau = \left(a_{kl}^{(\tau(k))}\right)$ whose k th row is given by the k th row of $\mathbf{A}_{\tau(k)}$. For a power index $(\alpha_1, \dots, \alpha_m)$ with $\alpha_i \in \{0, 1, \dots, d+J-1\}$ and $\sum_{i=1}^m \alpha_i = d+J-1$, we denote

$$\tau \in (\alpha_1, \dots, \alpha_m)$$

if $\alpha_i = \#\{j : \tau(j) = i\}$ for each $i = 1, \dots, m$. In terms of the construction of \mathbf{A}_τ , it says that α_i rows of \mathbf{A}_τ are from the matrix \mathbf{A}_i .

According to the Leibniz formula for the determinant,

$$|\mathbf{F}| = \left| \sum_{i=1}^m n_i \mathbf{A}_i \right| = \sum_{\sigma \in S_{d+J-1}} (-1)^{\text{sgn}(\sigma)} \prod_{k=1}^{d+J-1} \sum_{i=1}^m n_i a_{k, \sigma(k)}^{(i)}$$

where σ is a permutation of $\{1, 2, \dots, d+J-1\}$, and $\text{sgn}(\sigma)$ is the sign or

signature of σ . Therefore,

$$\begin{aligned}
c_{\alpha_1, \dots, \alpha_m} &= \sum_{\sigma \in S_{d+J-1}} (-1)^{\text{sgn}(\sigma)} \sum_{\tau \in (\alpha_1, \dots, \alpha_m)} \prod_{k=1}^{d+J-1} a_{k, \sigma(k)}^{(\tau(k))} \\
&= \sum_{\tau \in (\alpha_1, \dots, \alpha_m)} \sum_{\sigma \in S_{d+J-1}} (-1)^{\text{sgn}(\sigma)} \prod_{k=1}^{d+J-1} a_{k, \sigma(k)}^{(\tau(k))} \\
&= \sum_{\tau \in (\alpha_1, \dots, \alpha_m)} |\mathbf{A}_\tau|
\end{aligned}$$

□

Proof of Lemma 2.2 To simplify the notations, we let $i_s = s+1$, $s = 0, \dots, d$. That is, $\alpha_1 = J-1$, $\alpha_2 = \dots = \alpha_{d+1} = 1$. There are only two types of $\tau \in (\alpha_1, \dots, \alpha_m)$, such that, $|\mathbf{A}_\tau|$ may not be 0.

τ of type I: There exist $1 \leq k \leq d$, $2 \leq l \leq d+1$, and $1 \leq q \leq J-1$, such that, $\tau(k) = 1$ and $\tau(d+q) = l$. Following a similar procedure as in the proof of Lemma S.5, we obtain

$$|\mathbf{A}_\tau| = \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X}_1[1, 2, \dots, d+1]| \cdot (-1)^{\text{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s} \cdot \frac{c_l q}{e_l}$$

τ of type II: $\tau(d+1) = \dots = \tau(d+J-1) = 1$ and $\{\tau(1), \dots, \tau(d)\} = \{2, \dots, d+1\}$. It can be verified that

$$|\mathbf{A}_\tau| = \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X}_1[1, 2, \dots, d+1]| \cdot (-1)^{\text{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s}$$

According to Theorem 2.2,

$$\begin{aligned}
c_{\alpha_1, \dots, \alpha_m} &= \sum_{\tau \text{ of type I}} |\mathbf{A}_\tau| + \sum_{\tau \text{ of type II}} |\mathbf{A}_\tau| \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X}_1[1, 2, \dots, d+1]| \cdot \left(\sum_{k=1}^d \sum_{l=2}^{d+1} \sum_{\tau \in S_{d+1}: \tau(k)=1, \tau(d+1)=l} \right)
\end{aligned}$$

$$\begin{aligned}
& (-1)^{\text{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s} \sum_{q=1}^{J-1} \frac{c_{lq}}{e_l} + \sum_{\tau \in S_{d+1}: \tau(d+1)=1} (-1)^{\text{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s} \bigg) \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X}_1[1, 2, \dots, d+1]| \cdot \sum_{\tau \in S_{d+1}} (-1)^{\text{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s} \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X}_1[1, 2, \dots, d+1]| \cdot (-1)^d |\mathbf{X}_1[1, 2, \dots, d+1]| \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot |\mathbf{X}_1[1, 2, \dots, d+1]|^2
\end{aligned}$$

where S_{d+1} is the set of permutations of $\{1, \dots, d+1\}$. The general case with i_0, i_1, \dots, i_d can be obtained similarly. \square

Proof of Theorem 2.4 Suppose $\text{Rank}(\mathbf{X}_1) = d+1$. Then there exist $i_0, \dots, i_d \in \{1, \dots, m\}$, such that, $|\mathbf{X}_1[i_0, i_1, \dots, i_d]| \neq 0$. According to Lemma S.4, $f(\mathbf{p})$ can be regarded as an order- $(J-1)$ polynomial of p_{i_0} . Let $p_{i_0} = x \in (0, 1)$ and $p_i = (1-x)/(m-1)$ for $i \neq i_0$. Based on Lemma 2.2, $f(\mathbf{p})$ can be written as

$$\begin{aligned}
f_{i_0}(x) &= a_{J-1} x^{J-1} \left(\frac{1-x}{m-1} \right)^d + a_{J-2} x^{J-2} \left(\frac{1-x}{m-1} \right)^{d+1} \\
&\quad + \dots + a_1 x \left(\frac{1-x}{m-1} \right)^{d+J-2} + a_0 \left(\frac{1-x}{m-1} \right)^{d+J-1}, \text{ where} \\
a_{J-1} &= |\mathbf{A}_{i_0 3}| \sum_{\{i'_1, \dots, i'_d\} \subset \{1, \dots, m\} \setminus \{i_0\}} \prod_{s=1}^d e_{i'_s} |\mathbf{X}_1[i_0, i'_1, \dots, i'_d]|^2 > 0
\end{aligned}$$

Therefore, $\lim_{x \rightarrow 1^-} (1-x)^{-d} x^{1-J} f_{i_0}(x) = (m-1)^{-d} a_{J-1} > 0$. That is, $f(\mathbf{p}) > 0$ for $p_{i_0} = x$ close enough to 1 and $p_i = (1-x)/(m-1)$ for $i \neq i_0$.

In order to justify that the condition $\text{Rank}(\mathbf{X}_1) = d+1$ is also necessary, we only need to show that $f(\mathbf{p}) \equiv 0$ if $\text{Rank}(\mathbf{X}_1) \leq d$. Actually, for any $\tau : \{1, \dots, d+J-1\} \rightarrow \{1, \dots, m\}$, we construct $\mathbf{A}_\tau^{(1)}$ as in the proof of Lemma S.5. Then $|\mathbf{A}_\tau| = \prod_{s=1}^d x_{\tau(s)s} \cdot |\mathbf{A}_\tau^{(1)}|$. Similar as in the proof of Lemma S.5, for $t = 1, \dots, d$, we add $x_{\tau(1)t}(-e_{\tau(1)}, \dots, -e_{\tau(d)}, c_{\tau(d+1)1}, \dots, c_{\tau(d+J-1), J-1})^T$ to the t th column of $\mathbf{A}_\tau^{(1)}$. We denote the resulting matrix by $\mathbf{A}_\tau^{(3)}$. Note that $|\mathbf{A}_\tau^{(1)}| =$

$|\mathbf{A}_\tau^{(3)}|$. We consider the sub-matrix $\mathbf{A}_{\tau d}^{(3)}$ which consists of the first d columns of $\mathbf{A}_\tau^{(3)}$. For $s \in \tau^{-1}(\tau(1))$, the s th row of $\mathbf{A}_{\tau d}^{(3)}$ is simply 0. For $s = 2, \dots, k$, the s th row of $\mathbf{A}_{\tau d}^{(3)}$ is $e_{\tau(s)}(x_{\tau(s)1} - x_{\tau(1)1}, \dots, x_{\tau(s)d} - x_{\tau(1)d})$. For $s = 1, \dots, J-1$, the $(d+s)$ th row of $\mathbf{A}_{\tau d}^{(3)}$ is $-c_{\tau(d+s)}(x_{\tau(d+s)1} - x_{\tau(1)1}, \dots, x_{\tau(d+s)d} - x_{\tau(1)d})$. We claim that $\text{Rank}(\mathbf{A}_{\tau d}^{(3)}) \leq d-1$. Otherwise, if $\text{Rank}(\mathbf{A}_{\tau d}^{(3)}) = d$, then there exist $i_1, \dots, i_d \in \{2, \dots, d+J-1\}$, such that, the sub-matrix consisting of the i_1 th, \dots , i_d th rows of $\mathbf{A}_{\tau d}^{(3)}$ is nonsingular. Then the sub-matrix consisting of the $\tau(1)$ th, $\tau(i_1)$ th, \dots , $\tau(i_d)$ th rows of \mathbf{X}_1 is nonsingular, which implies $\text{Rank}(\mathbf{X}_1) = d+1$. The contradiction implies $\text{Rank}(\mathbf{A}_{\tau d}^{(3)}) \leq d-1$. Then $|\mathbf{A}_\tau^{(3)}| = 0$ and thus $|\mathbf{A}_\tau| = 0$ for each τ . Based on Theorem 2.2, $|\mathbf{F}| \equiv 0$ and thus $f(\mathbf{p}) \equiv 0$. \square

Proof of Theorem 3.5 Combining Theorem 2.1 and Theorem 2.4, it is straightforward that $f(\mathbf{p}) = 0$ if $\text{Rank}(\mathbf{X}_1[\{i \mid p_i > 0\}]) \leq d$. We only need to show that $f(\mathbf{p}) > 0$ if $\text{Rank}(\mathbf{X}_1[\{i \mid p_i > 0\}]) = d+1$. Due to Theorem 2.1, we only need to verify the case $p_i > 0, i = 1, \dots, m$. (Otherwise, we may simply remove all support points with $p_i = 0$.)

Suppose $p_i > 0, i = 1, \dots, m$ and $\text{Rank}(\mathbf{X}_1) = d+1$. Then there exist $i_0, \dots, i_d \in \{1, \dots, m\}$, such that, $|\mathbf{X}_1[i_0, \dots, i_d]| \neq 0$. According to the proof of Theorem 2.4, for each $i \in \{i_0, \dots, i_d\}$, there exists an $\epsilon_i \in (0, 1)$, such that, $f(\mathbf{p}) > 0$ as long as $p_i = x \in (1 - \epsilon_i, 1)$ and $p_j = (1 - x)/(m-1)$ for $j \neq i$. On the other hand, for each $i \notin \{i_0, \dots, i_d\}$, if we denote the j th row of \mathbf{X}_1 by α_j , $j = 1, \dots, m$, then $\alpha_i = a_0\alpha_{i_0} + \dots + a_d\alpha_{i_d}$ for some real numbers a_0, \dots, a_d . Since $\alpha_i \neq 0$, then at least one $a_i \neq 0$. Without any loss of generality, we assume $a_0 \neq 0$. Then it can be verified that $|\mathbf{X}_1[i, i_1, \dots, i_d]| \neq 0$ too. Following the proof of Theorem 2.4 again, for such an $i \notin \{i_0, \dots, i_d\}$, there also exists an $\epsilon_i \in (0, 1)$, such that, $f(\mathbf{p}) > 0$ as long as $p_i = x \in (1 - \epsilon_i, 1)$ and $p_j = (1 - x)/(m-1)$ for $j \neq i$. Let $\epsilon_* = \min\{\min_i \epsilon_i, (m-1) \min_i p_i, 1 - 1/m\}/2$. For $i = 1, \dots, m$, denote $\delta_i = (\delta_{i1}, \dots, \delta_{im})^T \in S$ with $\delta_{ii} = 1 - \epsilon_*$ and $\delta_{ij} = \epsilon_*/(m-1)$ for $j \neq i$. It can be verified that $\mathbf{p} = a_1\delta_1 + \dots + a_m\delta_m$ with $a_i = (p_i - \epsilon_*/(m-1))/(1 - m\epsilon_*/(m-1))$. By the choice of ϵ_* , $f(\delta_i) > 0, a_i > 0, i = 1, \dots, m$, and $\sum_i a_i = 1$. Then $f(\mathbf{p}) > 0$ according to Lemma S.6. \square

Proof of Corollary 5.3 In order to check when a minimally supported design supported only on $\{x_1, x_2\}$ is D-optimal, we add one more support point, that

is, x_3 . According to Theorem 2.2, Lemmas S.4, S.5, and 2.2, the objective function for a D-optimal approximate design on $\{x_1, x_2, x_3\}$ is $f(p_1, p_2, p_3) = p_1 p_2 (c_{210} p_1 + c_{120} p_2) + p_1 p_3 (c_{201} p_1 + c_{102} p_3) + p_2 p_3 (c_{021} p_2 + c_{012} p_3) + c_{111} p_1 p_2 p_3$, where

$$\begin{aligned}
c_{210} &= e_2 g_{11}^2 g_{12}^2 (\pi_{11} \pi_{12} \pi_{13})^{-1} (x_1 - x_2)^2 > 0 \\
c_{120} &= e_1 g_{21}^2 g_{22}^2 (\pi_{21} \pi_{22} \pi_{23})^{-1} (x_1 - x_2)^2 > 0 \\
c_{201} &= e_3 g_{11}^2 g_{12}^2 (\pi_{11} \pi_{12} \pi_{13})^{-1} (x_1 - x_3)^2 > 0 \\
c_{102} &= e_1 g_{31}^2 g_{32}^2 (\pi_{31} \pi_{32} \pi_{33})^{-1} (x_1 - x_3)^2 > 0 \\
c_{021} &= e_3 g_{21}^2 g_{22}^2 (\pi_{21} \pi_{22} \pi_{23})^{-1} (x_2 - x_3)^2 > 0 \\
c_{012} &= e_2 g_{31}^2 g_{32}^2 (\pi_{31} \pi_{32} \pi_{33})^{-1} (x_2 - x_3)^2 > 0 \\
c_{111} &= e_1 (u_{22} u_{31} + u_{21} u_{32} - 2b_{22} b_{32}) (x_1 - x_2) (x_1 - x_3) + \\
&\quad e_2 (u_{12} u_{31} + u_{11} u_{32} - 2b_{12} b_{32}) (x_2 - x_1) (x_2 - x_3) + \\
&\quad e_3 (u_{12} u_{21} + u_{11} u_{22} - 2b_{12} b_{22}) (x_3 - x_1) (x_3 - x_2)
\end{aligned}$$

Based on Theorem 5.10, the design $\mathbf{p} = (p_1^*, p_2^*, 0)^T$ is D-optimal if and only if

$$\partial f(\mathbf{p}) / \partial f(p_1) = \partial f(\mathbf{p}) / \partial f(p_2) \geq \partial f(\mathbf{p}) / \partial f(p_3)$$

Similar conclusions could be justified for x_4, \dots, x_m if $m \geq 4$. \square

Proof of Theorem 5.12 According to the solutions provided by the software **Mathematica**, the largest root of equation (S.10) after simplification is

$$y_1 = -\frac{b_2}{3} - \frac{2^{1/3}(3b_1 - b_2^2)}{3A^{1/3}} + \frac{A^{1/3}}{3 \times 2^{1/3}} \quad (\text{S.11})$$

where $A = -27b_0 + 9b_1b_2 - 2b_2^3 + 3^{3/2}(27b_0^2 + 4b_1^3 - 18b_0b_1b_2 - b_1^2b_2^2 + 4b_0b_2^3)^{1/2}$, and $b_i = c_i/c_3$, $i = 0, 1, 2$. Note that the calculation of A and thus y_1 should be regarded as operations among complex numbers since the expression under square root could be negative. Nevertheless, y_1 at the end would be a real number. Thus we are able to provide the analytic solution maximizing $f(p_1, p_2, p_3)$. \square

Proof of Corollary 5.5 In order to check when a minimally supported design is D-optimal, we first add the four design points, that is, we consider four design

points (x_{i1}, x_{i2}) , $i = 1, 2, 3, 4$ and check when the D-optimal design could be constructed on the first three design points. Let \mathbf{X}_1 be defined as in Lemma 2.2. In this case, \mathbf{X}_1 is a 4×3 matrix. Following Theorem 2.2, Lemmas S.4, S.5, and 2.2, the objective function for a minimally supported design at $(d, J, m) = (2, 3, 4)$ is

$$\begin{aligned} f(p_1, p_2, p_3, p_4) &= c_{1111} p_1 p_2 p_3 p_4 \\ &+ |\mathbf{X}_1[1, 2, 3]|^2 e_1 e_2 e_3 \cdot p_1 p_2 p_3 (w_1 p_1 + w_2 p_2 + w_3 p_3) \\ &+ |\mathbf{X}_1[1, 2, 4]|^2 e_1 e_2 e_4 \cdot p_1 p_2 p_4 (w_1 p_1 + w_2 p_2 + w_4 p_4) \\ &+ |\mathbf{X}_1[1, 3, 4]|^2 e_1 e_3 e_4 \cdot p_1 p_3 p_4 (w_1 p_1 + w_3 p_3 + w_4 p_4) \\ &+ |\mathbf{X}_1[2, 3, 4]|^2 e_2 e_3 e_4 \cdot p_2 p_3 p_4 (w_2 p_2 + w_3 p_3 + w_4 p_4) \end{aligned}$$

where $e_i = u_{i1} + u_{i2} - 2b_{i2}$, $w_i = e_i^{-1} g_{i1}^2 g_{i2}^2 (\pi_{i1} \pi_{i2} \pi_{i3})^{-1}$, $i = 1, 2, 3, 4$, and

$$c_{1111} = \sum_{1 \leq i < j \leq 4} e_i e_j (u_{k1} u_{l2} + u_{k2} u_{l1} - 2b_{k2} b_{l2}) \cdot |\mathbf{X}_1[i, j, k]| \cdot |\mathbf{X}_1[i, j, l]| \quad (\text{S.12})$$

with $\{i, j, k, l\} = \{1, 2, 3, 4\}$ given $1 \leq i < j \leq 4$.

According to Theorem 5.10, a minimally supported design $\mathbf{p} = (p_1^*, p_2^*, p_3^*, 0)^T$ in this case is D-optimal if and only if $\partial f / \partial p_1 = \partial f / \partial p_2 = \partial f / \partial p_3 \geq \partial f / \partial p_4$ at \mathbf{p} . Then $\partial f / \partial p_1 = \partial f / \partial p_2 = \partial f / \partial p_3$ at \mathbf{p} is equivalent to (1) of Corollary 5.5, and $\partial f / \partial p_4 \leq \partial f / \partial p_1$ at \mathbf{p} leads to (2) of Corollary 5.5 since the forms of $\partial f / \partial p_i$ at \mathbf{p} , $i = 1, 2, 3$ will not change if more than four design points (i.e., $m > 4$) are added into consideration. Note that

$|\mathbf{X}_1[1, 2, 3]|^2 e_1 e_2 e_3 p_2^* p_3^* (2w_1 p_1^* + w_2 p_2^* + w_3 p_3^*)$ in (2) of Corollary 5.5 is equal to $\partial f / \partial p_1$ at \mathbf{p} . It could be replaced with $|\mathbf{X}_1[1, 2, 3]|^2 e_1 e_2 e_3 p_1^* p_3^* (w_1 p_1^* + 2w_2 p_2^* + w_3 p_3^*)$ (i.e., $\partial f / \partial p_2$), or $|\mathbf{X}_1[1, 2, 3]|^2 e_1 e_2 e_3 p_1^* p_2^* (w_1 p_1^* + w_2 p_2^* + 2w_3 p_3^*)$ (i.e., $\partial f / \partial p_3$), since these three are all equal. \square

S.4 Maximization of $f_i(z)$ in Section 3

According to Theorem 3.6, $f_i(z)$ is an order- $(d+J-1)$ polynomial of z . In order to determine its coefficients a_0, a_1, \dots, a_{J-1} as in (3.2), we need to calculate $f_i(0)$, $f_i(1/2)$, $f_i(1/3)$, \dots , $f_i(1/J)$, which are J determinants defined in (3.1).

Note that \mathbf{B}_{J-1}^{-1} is a matrix determined by $J-1$ only. For example, $B_1^{-1} = 1$

for $J = 2$,

$$B_2^{-1} = \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}, B_3^{-1} = \begin{pmatrix} 3 & -3 & 1 \\ -\frac{5}{2} & 4 & -\frac{3}{2} \\ \frac{1}{2} & -1 & \frac{1}{2} \end{pmatrix},$$

$$B_4^{-1} = \begin{pmatrix} 4 & -6 & 4 & -1 \\ -\frac{13}{3} & \frac{19}{2} & -7 & \frac{11}{6} \\ \frac{3}{2} & -4 & \frac{7}{2} & -1 \\ -\frac{1}{6} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{6} \end{pmatrix}$$

for $J = 3, 4$, or 5 respectively.

Once a_0, \dots, a_{J-1} in (3.2) are determined, the maximization of $f_i(z)$ on $z \in [0, 1]$ is numerically straightforward since it is a polynomial and its derivative is given by

$$f'_i(z) = (1-z)^d \sum_{j=1}^{J-1} j a_j z^{j-1} (1-z)^{J-1-j} - (1-z)^{d-1} \sum_{j=0}^{J-1} (d+J-1-j) a_j z^j (1-z)^{J-1-j} \quad (\text{S.13})$$

S.5 Exchange algorithm for D-optimal exact allocation in Section 4

Exchange algorithm for D-optimal allocation $(n_1, \dots, n_m)^T$ given $n > 0$:

- 1° Start with an initial design $\mathbf{n} = (n_1, \dots, n_m)^T$ such that $f(\mathbf{n}) > 0$.
- 2° Set up a random order of (i, j) going through all pairs $\{(1, 2), (1, 3), \dots, (1, m), (2, 3), \dots, (m-1, m)\}$.
- 3° For each (i, j) , let $c = n_i + n_j$. If $c = 0$, let $\mathbf{n}_{ij}^* = \mathbf{n}$. Otherwise, there are two cases. *Case one:* $0 < c \leq J$, we calculate $f_{ij}(z)$ as defined in (4.1) for $z = 0, 1, \dots, c$ directly and find z^* which maximizes $f_{ij}(z)$. *Case two:* $c > J$, we first calculate $f_{ij}(z)$ for $z = 0, 1, \dots, J$; secondly determine c_0, c_1, \dots, c_J in (4.2) according to Theorem 4.9; thirdly calculate $f_{ij}(z)$ for $z = J+1, \dots, c$ based on (4.2); fourthly find z^* maximizing $f_{ij}(z)$ for $z = 0, \dots, c$. For both

cases, we define

$$\mathbf{n}_{ij}^* = (n_1, \dots, n_{i-1}, z^*, n_{i+1}, \dots, n_{j-1}, c - z^*, n_{j+1}, \dots, n_m)^T$$

Note that $f(\mathbf{n}_{ij}^*) = f_{ij}(z^*) \geq f(\mathbf{n}) > 0$. If $f(\mathbf{n}_{ij}^*) > f(\mathbf{n})$, replace \mathbf{n} with \mathbf{n}_{ij}^* , and $f(\mathbf{n})$ with $f(\mathbf{n}_{ij}^*)$.

4° Repeat 2° \sim 3° until convergence, that is, $f(\mathbf{n}_{ij}^*) = f(\mathbf{n})$ in step 3° for any (i, j) .

S.6 More on Example 4.6: Polysilicon Deposition Study

Table S.1 shows the list of experimental settings for the polysilicon deposition study. The factors are `decomposition temperature(A)`, `decomposition pressure(B)`, `nitrogen flow(C)`, `silane flow(D)`, `setting time(E)`, `cleaning method(F)`. Column 1 provides original indices of experimental settings out of 729 distinct ones. For each experimental setting labelled “1” in a design, 9 responses are collected (Phadke, 1989) and assumed to be independent.

Table S.2 shows the model matrix for the D-optimal design \mathbf{n}_o found for the polysilicon deposition study. In this table, each 3-level factor is represented by its linear component and quadratic component. Thus there are level combinations of 12 predictors.

Table S.1: Polysilicon Deposition Study: Experimental Settings for the Original Design, Rounded Approximate Design and D-optimal Exact Design

Index	A	B	C	D	E	F	Original	Rounded	D-optimal
1	1	1	1	1	1	1	1	0	0
76	1	1	3	3	2	1	1	0	0
89	1	2	1	1	3	2	1	0	0
98	1	2	1	2	3	2	0	0	1
111	1	2	2	1	1	3	0	0	1
116	1	2	2	1	3	2	0	1	0
122	1	2	2	2	2	2	1	0	0
130	1	2	2	3	2	1	0	0	1
167	1	3	1	1	2	2	0	0	1
181	1	3	1	3	1	1	0	1	0
199	1	3	2	2	1	1	0	1	1
201	1	3	2	2	1	3	1	0	0
243	1	3	3	3	3	3	1	0	1
258	2	1	1	2	2	3	1	0	0
286	2	1	2	2	3	1	0	1	0
290	2	1	2	3	1	2	1	0	0
291	2	1	2	3	1	3	0	1	0
294	2	1	2	3	2	3	0	0	1
299	2	1	3	1	1	2	0	0	1
301	2	1	3	1	2	1	0	1	0
313	2	1	3	2	3	1	0	0	1
331	2	2	1	1	3	1	0	1	1
336	2	2	1	2	1	3	0	1	1
339	2	2	1	2	2	3	0	1	0
350	2	2	1	3	3	2	0	1	0
365	2	2	2	2	2	2	0	0	1
376	2	2	2	3	3	1	1	0	0
384	2	2	3	1	2	3	1	0	0
394	2	2	3	2	3	1	0	1	0
399	2	2	3	3	1	3	0	1	0
407	2	3	1	1	1	2	0	0	1
421	2	3	1	2	3	1	1	0	0
461	2	3	3	1	1	2	1	1	0
464	2	3	3	1	2	2	0	1	0
495	3	1	1	1	3	3	0	1	0
501	3	1	1	2	2	3	0	0	1
505	3	1	1	3	1	1	0	0	1
521	3	1	2	1	3	2	0	0	1
522	3	1	2	1	3	3	1	0	0
536	3	1	2	3	2	2	0	1	0
557	3	1	3	2	3	2	1	0	0
558	3	1	3	2	3	3	0	1	0
569	3	2	1	1	1	2	0	1	0
588	3	2	1	3	1	3	1	0	0
625	3	2	3	1	2	1	0	0	1
631	3	2	3	2	1	1	1	0	0
641	3	2	3	3	1	2	0	0	1
671	3	3	1	3	2	2	1	0	0
679	3	3	2	1	2	1	1	0	0

Table S.2: Polysilicon Deposition Study: Model Matrix for the D-optimal Design

Index	A_1	A_2	B_1	B_2	C_1	C_2	D_1	D_2	E_1	E_2	F_1	F_2
98	-1	1	0	-2	-1	1	0	-2	1	1	0	-2
111	-1	1	0	-2	0	-2	-1	1	-1	1	1	1
130	-1	1	0	-2	0	-2	1	1	0	-2	-1	1
167	-1	1	1	1	-1	1	-1	1	0	-2	0	-2
199	-1	1	1	1	0	-2	0	-2	-1	1	-1	1
243	-1	1	1	1	1	1	1	1	1	1	1	1
294	0	-2	-1	1	0	-2	1	1	0	-2	1	1
299	0	-2	-1	1	1	1	-1	1	-1	1	0	-2
313	0	-2	-1	1	1	1	0	-2	1	1	-1	1
331	0	-2	0	-2	-1	1	-1	1	1	1	-1	1
336	0	-2	0	-2	-1	1	0	-2	-1	1	1	1
365	0	-2	0	-2	0	-2	0	-2	0	-2	0	-2
407	0	-2	1	1	-1	1	-1	1	-1	1	0	-2
501	1	1	-1	1	-1	1	0	-2	0	-2	1	1
505	1	1	-1	1	-1	1	1	1	-1	1	-1	1
521	1	1	-1	1	0	-2	-1	1	1	1	0	-2
625	1	1	0	-2	1	1	-1	1	0	-2	-1	1
641	1	1	0	-2	1	1	1	1	-1	1	0	-2